

MATERIALS RESEARCH SOCIETY OF SERBIA  
INSTITUTE OF TECHNICAL SCIENCES OF SASA

*Programme and the Book of Abstracts*

**NINETEENTH YOUNG RESEARCHERS' CONFERENCE  
MATERIALS SCIENCE AND ENGINEERING**

Belgrade, December 1-3, 2021



**NINETEENTH YOUNG RESEARCHERS' CONFERENCE  
MATERIALS SCIENCE AND ENGINEERING**

**December 1-3, 2021, Belgrade, Serbia**

**Program and the Book of Abstracts**

**Materials Research Society of Serbia  
&  
Institute of Technical Sciences of SASA**

**2021**

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## Aim of the Conference

Main aim of the conference is to enable young researchers (post-graduate, master or doctoral student, or a PhD holder younger than 35) working in the field of materials science and engineering, to meet their colleagues and exchange experiences about their research.

## Topics

Biomaterials  
Environmental science  
Materials for high-technology applications  
Materials for new generation solar cells  
Nanostructured materials  
New synthesis and processing methods  
Theoretical modelling of materials

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**Results of the Conference**

Beside printed «Program and the Book of Abstracts», which is disseminated to all conference participants, selected and awarded peer-reviewed papers will be published in journal “Tehnika – Novi Materijali”. The best presented papers, suggested by Session Chairpersons and selected by Awards Committee, will be proclaimed at the Closing Ceremony. Part of the award is free-of-charge conference fee at YUCOMAT 2022.

**Sponsors**



**ANALYSIS**  
LABORATORY EQUIPMENT

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**Programme**  
**Nineteenth Young Researchers Conference**  
**Materials Science and Engineering**

**Wednesday, December 1, 2021**

**09.00 – 10.15 1<sup>st</sup> Session – Biomaterials I**

**Chairpersons: Prof. Dr. Bojana Obradović and Marija Kostić**

**09.00 – 09.15 Synthesis and characterization of the pH-sensitive saccharide-based polyurethane hydrogels**

Marija Kostić

*Faculty of Technology Novi Sad, University of Novi Sad, Novi Sad, Serbia*

**09.15 – 09.30 Antiradical activity of graphene quantum dots enriched albumin hydrogel: An EPR study**

Đura Nakarada<sup>1</sup>, Vladimir Trajković<sup>2</sup>, Miloš Mojović<sup>1</sup>

*<sup>1</sup>University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia, <sup>2</sup>University of Belgrade, Faculty of Medicine, Belgrade, Serbia*

**09.30 – 09.45 Characteristics of thin films of biological substances deposited on polyethylene terephthalate (PET) in terms of biomedical applications**

K. Szafran<sup>1</sup>, M. Jurak<sup>1</sup>, R. Mroccka<sup>2</sup>, A.E. Wiącek<sup>1</sup>

*<sup>1</sup>Department of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, POLAND, <sup>2</sup>Laboratory of X-Ray Optics, Centre for Interdisciplinary Research, Faculty of Science and Health, The John Paul II Catholic University of Lublin, Poland*

**09.45 – 10.00 Additive-free resveratrol micro- and nanoparticles and assessment of their toxicity**

Nina Tomić<sup>1</sup>, Maja Kuzmanović<sup>1</sup>, Dragana Mitić Ćulafić<sup>2</sup>, Magdalena M. Stevanović<sup>1</sup>

*<sup>1</sup>Institute of Technical Sciences of SASA, Knez Mihailova 35/IV 11000 Belgrade, Serbia, <sup>2</sup>Department of Microbiology, University of Belgrade - Faculty of Biology, Studentski trg 16, Belgrade, Serbia*

**10.00 – 10.15 The use of Langmuir's technique to assess the antibacterial properties of chemical substances**

Agata Ładniak<sup>1</sup>, Małgorzata Jurak<sup>1</sup>, Marta Palusińska-Szys<sup>2</sup>, Klaudia Woźniak<sup>1</sup>, Kacper Przykaza<sup>1</sup>, Agnieszka Ewa Wiącek<sup>1</sup>

*<sup>1</sup>Institute of Chemical Sciences, Department of Interfacial Phenomena, Faculty of Chemistry, Maria Curie-Skłodowska University, M. Curie-Skłodowska Sq. 3, 20-031 Lublin, Poland,*

<sup>2</sup>*Institute of Biological Sciences, Department of Genetics and Microbiology, Faculty of Biology and Biotechnology, Maria Curie-Skłodowska University, Akademicka 19, 20-033 Lublin, Poland*

## **10.15 – 10.30 Break**

### **10.30 – 12.00 2<sup>nd</sup> Session – Biomaterials II**

**Chairpersons: Dr. Djordje Veljović and Ivana Banićević**

#### **10.30 – 10.45 Development of a physiologically relevant 3D *in vitro* model for osteosarcoma cell cultivation comprising alginate composite scaffolds and a perfusion bioreactor system**

Ivana Banićević<sup>1</sup>, Mia Radonjić<sup>1</sup>, Marija Pavlović<sup>1</sup>, Milena Milivojević<sup>2</sup>, Milena Stevanović<sup>2,3,4</sup>, Jasmina Stojkovska<sup>1,5</sup>, Bojana Obradović<sup>1</sup>

<sup>1</sup>*Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia,* <sup>2</sup>*Institute of Molecular Genetics and Genetic Engineering, University of Belgrade, Belgrade, Serbia,* <sup>3</sup>*Faculty of Biology, University of Belgrade, Belgrade, Serbia,* <sup>4</sup>*Serbian Academy of Sciences and Arts, Belgrade, Serbia,* <sup>5</sup>*Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia*

#### **10.45 – 11.00 Electrochemical composite bioceramic coatings based on hydroxyapatite, chitosan and polyvinyl alcohol loaded with gentamicin**

Nevena Jaćimović<sup>1</sup>, Marija Došić<sup>2</sup>, Ana Janković<sup>1</sup>, Vesna Mišković – Stanković<sup>1</sup>

<sup>1</sup>*Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, Belgrade, Serbia,* <sup>2</sup>*Institute for Technology of Nuclear and Other Mineral Raw Materials, Bulevar Franš d'Eperea 86, Belgrade, Serbia*

#### **11.00 – 11.15 Optimization of Bioreactor Cultures of Glioblastoma Cells Immobilized in Alginate Microfibers**

Jelena Petrović<sup>1,2</sup>, Mia Radonjić<sup>1,2</sup>, Jasmina Stojkovska<sup>1,2</sup>, Bojana Obradović<sup>1</sup>

<sup>1</sup>*Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia,* <sup>2</sup>*Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia*

#### **11.15 – 11.30 Laser induced periodic surface structures on Ti thin films by ultrafast laser irradiation**

Nevena Božinović<sup>1</sup>, Vladimir Rajić<sup>1</sup>, Danilo Kisić<sup>1</sup>, Dragana Tošić<sup>1</sup>, Dubravka Milovanović<sup>2</sup>, Suzana Petrović<sup>1</sup>

<sup>1</sup>*Department of Atomic Physics, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, P.O. Box 522, 11001 Belgrade, University of Belgrade, Serbia;*

<sup>2</sup>*University of Belgrade, Institute of General and Physical Chemistry, Studentski trg 12/V, 11158 Belgrade, Serbia*

**11.30 – 11.45 Omitting mischmetal and zirconium as a next step in the development of biodegradable magnesium implants**

Maria Zemkova<sup>1</sup>, Peter Minarik<sup>1</sup>, Eva Jablonska<sup>2</sup>, Jozef Vesely<sup>1</sup>, Jan Bohlen<sup>3</sup>, Robert Kral<sup>1</sup>  
<sup>1</sup>Charles University, Ke Karlovu 5, 121 16 Prague, Czech Republic, <sup>2</sup>University of Chemistry and Technology, Technická 5, 166 28 Prague, Czech Republic, <sup>3</sup>Helmholtz-Zentrum Geesthacht, Magnesium Innovation Center, Max-Planck-Straße 1, 215 02 Geesthacht, Germany

**11.45 – 12.00 Photo-activation of a dental composite from within using optical fibers – a holographic study**

Evgenije Novta<sup>1</sup>, Tijana Lainović<sup>1</sup>, Dušan Grujić<sup>2</sup>, Svetlana Savić-Šević<sup>2</sup>, Dejan Pantelić<sup>2</sup>, Larisa Blažić<sup>1,3</sup>  
University of Novi Sad, Faculty of Medicine, School of Dental Medicine, Novi Sad, Serbia, University of Belgrade, Institute of Physics, Belgrade, Serbia, Dental Clinic of Vojvodina, Novi Sad, Serbia

**12.00 – 12.15 Break**

**12.15 – 13.30 3<sup>rd</sup> Session – Biomaterials III**

**Chairpersons: Dr. Magdalena Stevanović and Tamara Matić**

**12.15 – 12.30 Electrophoretic deposition vs. dip-coating of the bioceramic layers on Ti6Al4V scaffolds**

Marija Milivojević<sup>1</sup>, Željko Radovanović<sup>1</sup>, Suzana Dimitrijević<sup>2</sup>, Miljana Popović<sup>2</sup>, Rada Petrović<sup>2</sup>, Đorđe Veljović<sup>2</sup>, Đorđe Janačković<sup>2</sup>  
<sup>1</sup>Innovation Center of Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>2</sup>Faculty of Technology and Metallurgy University of Belgrade

**12.30 – 12.45 Dental inserts based on calcium hydroxyapatite: The influence of cation doping**

Tamara Matić<sup>1</sup>, Maja Ležaja Zebić<sup>2</sup>, Vesna Miletić<sup>3</sup>, Rada Petrović<sup>4</sup>, Đorđe Janačković<sup>4</sup>, Đorđe Veljović<sup>4</sup>  
<sup>1</sup>University of Belgrade, Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>2</sup>University of Belgrade, School of Dental Medicine, Belgrade, Serbia, <sup>3</sup>The University of Sydney, Faculty of Medicine and Health, Sydney Dental School, Surry Hills NSW, Australia, <sup>4</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

**12.45 – 13.00 Synthesis and antimicrobial properties of ZnO deposited on hydroxyapatite**

Marija Stevanović<sup>1</sup>, Rada Petrović<sup>2</sup>, Đorđe Veljović<sup>2</sup>, Suzana Dimitrijević<sup>2</sup>, Đorđe Janačković<sup>2</sup>



<sup>1</sup>*Inovacioni Centar Tehnološko-metalurškog fakulteta u Beogradu d.o.o.*, <sup>2</sup>*Tehnološko-metalurški fakultet Univerziteta u Beogradu*

**13.00 – 13.15 Processing of gelatine coated composite scaffolds based on magnesium and strontium doped hydroxyapatite and yttria-stabilised zirconium oxide**

Aleksa Galić<sup>1</sup>, Tamara Matić<sup>2</sup>, Nataša Obradović<sup>2</sup>, Đorđe Veljović<sup>1</sup>

<sup>1</sup>*University of Belgrade, Faculty of Technology and Metallurgy, Department of Inorganic Chemical Technologies, Karnegijeva 4, 11000 Belgrade, Serbia*, <sup>2</sup>*Innovation Center of Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Belgrade, Serbia*

**13.15 – 13.30 Dissolving and water absorption ability of spray-dried willow gentian extract**

Miloš Jovanović<sup>1</sup>, Nada Čujić-Nikolić<sup>1</sup>, Zorica Drinić<sup>1</sup>, Teodora Janković<sup>1</sup>, Smilja Marković<sup>2</sup>, Katarina Šavikin<sup>1</sup>

<sup>1</sup>*Institute for Medicinal Plants Research “Dr. Josif Pančić”, Tadeuša Košćuška 1, 11000 Belgrade*, <sup>2</sup>*Institute of Technical Sciences of SASA, Knez Mihailova 35/IV, 11000 Belgrade*

**13.30 – 14.45 Lunch break**

**14.45 – 16.15 4<sup>th</sup> Session – Environmental Materials I**

**Chairpersons: Dr. Smilja Marković and Dr. Konrad Terpiłowski**

**14.45 – 15.00 Hydrophobization, a method of monument protection**

Joanna Podkościelna, Konrad Terpiłowski

*Department of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie Skłodowska University Lublin, Poland*

**15.00 – 15.15 Optimization of biodiesel production from waste cooking oil using waste-based CaO/zeolite catalyst**

Stefan Pavlović, Dalibor Marinković, Miroslav Stanković

*University of Belgrade, Institute of Chemistry, Technology, and Metallurgy-National Institute of Republic of Serbia, Njegoševa 12, 11000 Belgrade*

**15.15 – 15.30 Experimental determination of thermodynamic properties and modeling of new choline based ionic liquids**

Ivona Đorđević, Nikola Grozdanić, Ivona Radović

*University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia*

**15.30 – 15.45 Xylanase production from *Penicillium chrysogenum* and its application in degradation of agricultural waste**

Olivera Vukoičić, Nataša Šekuljica, Zorica Knežević-Jugović

*University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia*

**15.45 – 16.00 Carbon material derived from viscose as adsorbent for chlorpyrifos**

Vedran Milanković<sup>1</sup>, Tamara Lazarević – Pašti<sup>2</sup>

<sup>1</sup>*University of Belgrade, Faculty of Physical Chemistry, Studentski Trg 12, 11000 Belgrade, Serbia,* <sup>2</sup>*University of Belgrade, VINČA Institute of Nuclear Sciences - National Institute of the Republic of Serbia, Mike Petrovica Alasa 12-14, 11000 Belgrade, Serbia.*

**16.00 – 16.15 Application of DInSAR Technology for Monitoring the Subsidence Induced by Salt Mining in Tuzla, Bosnia and Herzegovina**

Bojana Grujić, Žarko Grujić

*University of Banja Luka, Faculty of Architecture, Civil Engineering and Geodesy, Banja Luka /Department of Civil Engineering*

**16.15 – 16.30 Break**

**16.30 – 18.00 5<sup>th</sup> Session – Environmental Materials II**

**Chairpersons: Dr. Ana Stanković and Michał Chodkowski**

**16.30 – 16.45 Effective sorption of toxic brilliant green using lignocellulosic waste biomasses and derived biochar samples**

Anja Antanasković<sup>1</sup>, Zorica Lopičić<sup>1</sup>, Tatjana Šoštarić<sup>1</sup>, Jelena Milojković<sup>1</sup>, Vladimir Adamović<sup>1</sup>, Kristina Vučković<sup>2</sup>, Milan Milivojević<sup>2</sup>

<sup>1</sup>*Institute for Technology of Nuclear and Other Mineral Raw Materials, Belgrade, Serbia,*

<sup>2</sup>*Faculty of Technology and Metallurgy, University of Belgrade, Serbia*

**16.45 – 17.00 Synthesis of Samarium and Zirconium-doped TiO<sub>2</sub> nanofibers with improved photocatalytic activity**

Sanita Ahmetović<sup>1</sup>, Zorka Ž. Vasiljević<sup>1</sup>, Nikola Cvjetičanin<sup>2</sup>, Jelena Vujančević<sup>3</sup>, Nenad B. Tadić<sup>4</sup>, Vladimir B. Pavlović<sup>5</sup>, Maria Vesna Nikolić<sup>1</sup>

<sup>1</sup>*University of Belgrade – Institute for Multidisciplinary Research, Belgrade, Serbia,*

<sup>2</sup>*University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia,* <sup>3</sup>*ITS SASA,*

*Belgrade, Serbia,* <sup>4</sup>*University of Belgrade, Faculty of Agriculture, Belgrade, Serbia*

**17.00 – 17.15 Investigation of biological activity of freeze-dried goat whey with the addition of dry spices**

Mihailo Mladenović, Marija Milić, Suzana Dimitrijević-Branković

*University of Belgrade, Faculty of Technology and Metallurgy, Department of Biochemical Engineering and Biotechnology*

**17.15 – 17.30 Europium-doped manganese tungstate for dual electrocatalytic activity**

Andrej Kukuruzar<sup>1</sup>, Slađana Savić<sup>1</sup>, Filip Vlahović<sup>2</sup>, Dalibor Stanković<sup>1,3</sup>

<sup>1</sup>University of Belgrade, Faculty of Chemistry, Studentski trg 12-16, 11000, Beograd, Serbia,

<sup>2</sup>Innovation Center of the Faculty of Chemistry, University of Belgrade, Serbia, <sup>3</sup>'VINČA' Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia

### **17.30 – 17.45 Thermally activated pyrophyllite as ceramic membrane**

Katarina Tošić<sup>1</sup>, Bojana Paskaš Mamula<sup>1</sup>, Nikola Novaković<sup>1</sup>, Mirjana Medić Ilić<sup>1</sup>, Igor Milanović<sup>1</sup>, Silvana Dimitrijević<sup>2</sup>, Jasmina Grbović Novaković<sup>1</sup>

<sup>1</sup>Centre of Excellence for Hydrogen and Renewable Energy, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, POB 522 Belgrade, Serbia, <sup>2</sup>The Mining and Metallurgy Institute Bor, Zeleni bulevar 35, 19210 Bor, Serbia

### **17.45 – 18.00 Effects of sulphur hexafluoride cold plasma hydrophobization on the polyoxymethylene surface**

Michał Chodkowski<sup>1</sup>, Zoltan Károly<sup>2</sup>, Szilvia Klébert<sup>2</sup>, Konrad Terpiłowski<sup>1</sup>

<sup>1</sup>Department of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Skłodowska University in Lublin (UMCS), pl. Marii Curie-Skłodowskiej 3, 20-031 Lublin, Poland, <sup>2</sup>Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Magyar tudósok körútja 2, H-1117 Budapest, Hungary

**Thursday, December 2, 2021**

**09.00 – 10.30 6<sup>th</sup> Session – Nanostructured Materials I**

**Chairpersons: Dr. Sonja Jovanović and Dr. Ivana Dinić**

**09.00 – 09.15 Effect of processing parameters on NaGdYF<sub>4</sub>:Yb,Er UCNPs structural, morphological and optical properties**

Ivana Dinić<sup>1</sup>, Marina Vuković<sup>2</sup>, Marko Nikolic<sup>3</sup> and Lidija Mancić<sup>1</sup>

<sup>1</sup>*Institute of Technical Sciences of SASA, Belgrade, Serbia*, <sup>2</sup>*Innovative Centre, Faculty of Chemistry Belgrade, University of Belgrade, Serbia*, <sup>3</sup>*Photonic Center, Institute of Physics Belgrade, University of Belgrade, Serbia*

**09.15 – 09.30 Electrochemical synthesis of silver nanoparticles in poly(vinyl alcohol)-based hydrogels and evaluation of their sizes by comparing experimental and simulated UV-visible spectra**

Marko Opsenica, Katarina Nešović, Vesna Mišković-Stanković

*University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia*

**09.30 – 09.45 Radiation-chemical synthesis of antibacterial Ag-poly(vinyl alcohol)/poly(N-vinyl-2-pyrrolidone) nanocomposite hydrogels**

Nikolina Nikolić, Jelena Spasojević, Aleksandra Radosavljević, Zorica Kačarević-Popović  
*Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*

**09.45 – 10.00 Synthesis of nano-sized NiMn<sub>2</sub>O<sub>4</sub> by glycine nitrate and electrospinning processes and its pseudocapacitive behavior**

Milena Dojčinović<sup>1</sup>, Zorka Ž. Vasiljević<sup>1</sup>, Nenad Tadić<sup>2</sup>, Jugoslav Krstić<sup>3</sup>, Smilja Marković<sup>4</sup>, Matiaž Spreitzer<sup>5</sup>, Janez Kovač<sup>5</sup>, Maria Vesna Nikolić<sup>1</sup>

<sup>1</sup>*University of Belgrade – Institute for Multidisciplinary Research, Belgrade, Serbia*,

<sup>2</sup>*University of Belgrade, Faculty of Physics, Belgrade, Serbia*, <sup>3</sup>*University of Belgrade*,

*ICH<sub>TM</sub>, Belgrade, Serbia*, <sup>4</sup>*ITS of SASA, Belgrade, Serbia*, <sup>5</sup>*Institute Jožef Štefan, Ljubljana, Slovenia*

**10.00 – 10.15 Characterization of a new Yb<sup>3+</sup>/Er<sup>3+</sup> doped SrGd<sub>2</sub>O<sub>4</sub> up-conversion nanomaterial obtained via glycine-assisted combustion synthesis**

Tijana Stamenković<sup>1</sup>, Nadežda Radmilović<sup>1</sup>, Marija Prekajski-Dorđević<sup>2</sup>, Ivana Dinić<sup>3</sup>, Lidija Mančić<sup>3</sup>, Vesna Lojpur<sup>1</sup>

<sup>1</sup>*Department of Atomic Physics, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, P.O. Box 522, 11001 Belgrade, University of Belgrade, Serbia*,

<sup>2</sup>*Department of Materials, Vinča Institute of Nuclear Sciences, National Institute of the*



*Republic of Serbia, P.O. Box 522, 11001 Belgrade, University of Belgrade, Serbia, <sup>3</sup>Institute of Technical Science of SASA, Knez-Mihailova 35/4, Belgrade, Serbia*

**10.15 – 10.30 Improving the compatibility of zirconium oxide nanoparticles and styrene-free polyester resin by coupling with vinyl functionalized silane**

Jelena D. Gržetić<sup>1</sup>, Slavko Mijatov<sup>1</sup>, Marica Bogosavljević<sup>1</sup>, Tihomir Kovačević<sup>1</sup>, Saša Brzić<sup>1</sup>

*Military Technical Institute, Ratka Resanovića 1, Belgrade, Serbia*

**10.30 – 10.45 Break**

**10.45 – 12.30 7<sup>th</sup> Session – Nanostructured Materials II**  
**Chairpersons: Dr. Suzana Filipović and Željko Mravik**

**10.45 – 11.00 Graphene quantum dots with amino groups as a potential photoluminescent probe for Fe(III) ions**

Sladana Dorončić<sup>1</sup>, Olivera Marković<sup>2</sup>, Duška Kleut<sup>1</sup> and Svetlana Jovanović<sup>1</sup>

*<sup>1</sup>Vinča”-Institute of Nuclear sciences - National Institute of the Republic of Serbia, University of Belgrade P.O. Box 522, 11001 Belgrade, Serbia, <sup>2</sup>University of Belgrade-Institute of Chemistry, Technology and Metallurgy, Department of Chemistry, Njegoševa 12, 11000 Belgrade, Republic of Serbia*

**11.00 – 11.15 Nanocomposite graphene oxide/silver nanowires: structural and morphological analysis**

Aleksandra Mišović<sup>1</sup>, Danica Bajuk Bogdanović<sup>2</sup>, Milica Budimir<sup>1</sup> and Svetlana Jovanović<sup>1</sup>

*<sup>1</sup>”Vinča” Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, 11000 Belgrade, Serbia, <sup>2</sup>Faculty of Physical Chemistry, University of Belgrade, 11158 Belgrade, Serbia*

**11.15 – 11.30 Investigation of the interaction of graphene oxide and 12-tungstophosphoric acid in aqueous suspensions**

Milica Pejčič<sup>1</sup>, Željko Mravik<sup>1</sup>, Danica Bajuk-Bogdanović<sup>2</sup>, Snežana Uskoković-Marković<sup>3</sup>, Bojana Nedić Vasiljević<sup>2</sup>, Sonja Jovanović<sup>1</sup>, Zoran Jovanović<sup>1</sup>

*<sup>1</sup>Laboratory of Physics, Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia, <sup>2</sup>Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, <sup>3</sup>Faculty of Pharmacy, University of Belgrade, Belgrade, Serbia*

**11.30 – 11.45 Surface, structural and electric properties of ion beam irradiated graphene oxide papers**

Željko Mravik<sup>1</sup>, Marko Gloginjić<sup>1</sup>, Danica Bajuk-Bogdanović<sup>2</sup>, Maria Vesna Nikolić<sup>3</sup>, Andrej Olejniczak<sup>4,5</sup>, Nemanja Gavrilov<sup>2</sup>, Zoran Jovanović<sup>1</sup>

<sup>1</sup>*Center of Excellence for Hydrogen and Renewable Energy (CONVINCE), Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia,*

<sup>2</sup>*Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia,* <sup>3</sup>*Institute for Multidisciplinary Research, University of Belgrade, Serbia,* <sup>4</sup>*Flerov Laboratory of Nuclear Reactions, Joint Institute for Nuclear Research, Dubna, Moscow region, Russia,*

<sup>5</sup>*Faculty of Chemistry, Nicolaus Copernicus University, Toruń, Poland*

**11.45 – 12.00 Hydrothermal synthesis and characterization of composite of graphene oxide and cobalt ferrite doped with zink and gallium**

Marija Grujičić<sup>1,2</sup>, Ivana Stojković Simatović<sup>1</sup>, Danica Bajuk Bogdanović<sup>1</sup>, Zoran Jovanović<sup>2</sup>, Željko Mravik<sup>2</sup>, Sonja Jovanović<sup>2</sup>

<sup>1</sup>*Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia,* <sup>2</sup>*“VINČA” Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*

**12.00 – 12.15 Hybrid functional porous polymers, based on phosphazene and cage-like siloxane building blocks**

Mikhail Soldatov<sup>1</sup>, Anna Chernysheva<sup>1</sup>, Hongzhi Liu<sup>2</sup>, Sergei Kostjuk<sup>3</sup>

<sup>1</sup>*D. Mendeleev University of Chemical Technology of Russia, Moscow, Russian Federation,*

<sup>2</sup>*Shandong University, Jinan, People Republic of China,* <sup>3</sup>*Belarussian State University, Minsk, Republic of Belarus*

**12.15 – 12.30 Recent Progress of Carbon Dots in Nanomedicine and Photocatalysis**

Yiqun Zhou and Roger M. Leblanc

*University of Miami, USA*

**12.30 – 13.45 Lunch break**

**13.45 – 15.00 8<sup>th</sup> Session – Theoretical Modeling of Materials I**

**Chairpersons: Dr. Miloš Milović and Marko Jelić**

**13.45 – 14.00 Structural, spectroscopic and quantum-chemical investigation of testosterone propionate**

Nikola Ristivojević, Dušan Dimić

*University of Belgrade-Faculty of Physical Chemistry, Studentski trg 12-16, 11000 Belgrade, Serbia*

**14.00 – 14.15 Spectroscopic and theoretic analysis of hydrocortisone – forensic aspects**

Andjela Gavran, Dusan Dimic

*University of Belgrade-Faculty of Physical Chemistry, Studentski trg 12-16, 11000 Belgrade, Serbia*

**14.15 – 14.30 The role of defects in graphene for removal of toxic compounds – Theoretical analysis**

Marko Jelić<sup>1,2</sup>, Aleksandar Jovanović<sup>1</sup>, Igor Pašti<sup>1</sup>

<sup>1</sup>*Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, 2Laboratory of Physics, Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*

**14.30 – 14.45 A DFT study of the influence of chemical environment and boron concentration in boron-doped graphene on its reactivity**

Milica S. Ritopečki, Ana S. Dobrota

*University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia*

**14.45 – 15.00 Significant modulation of charge-transfer states properties in the biological assembly of the d(TG<sub>4</sub>T) sequence in crystal form**

Branislav Milovanović, Milena Petković, Mihajlo Etinski

*University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia*

**15.00 – 15.15 Break**

**15.15 – 16.45 9<sup>th</sup> Session – Theoretical Modeling of Materials II  
Chairpersons: Dr. Marko Opačić and Jovana Vlahović**

**15.15 – 15.30 Nitrogen-doped graphene nanoribbons: DFT prospects for Al-ion battery application**

Jovana Vlahović<sup>1,2</sup>, Ana S. Dobrota<sup>1</sup>, Natalia V. Skorodumova<sup>3,4</sup>, Igor A. Pašti<sup>1,3</sup>

<sup>1</sup>*University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia, 2University of Belgrade, Vinča Institute of Nuclear Sciences, Laboratory of Physics, Belgrade, Serbia, 3KTH-Royal Institute of Technology, School of Industrial Engineering and Management, Department of Materials Science and Engineering, Brinellvägen 23, Stockholm, 100 44, Sweden, 4Uppsala University, Department of Physics and Astronomy, Box 516, 751 20 Uppsala, Sweden*

**15.30 – 15.45 The possibility of achieving bound states in complex periodic potential of the Kronig-Penney type**

Jovana Obradović, Jelena Radovanović, Vitomir Milanović

*School of Electrical Engineering, University of Belgrade, Bulevar kralja Aleksandra 73, 11120 Belgrade, Serbia*

**15.45 – 16.00 Comparison of numerical methods for solving the effective mass Schrödinger equation for multilayer heterostructure applications**

Novak Stanojević, Jelena Radovanović, Vitomir Milanović

*School of Electrical Engineering, University of Belgrade, Bulevar kralja Aleksandra 73,  
11120 Belgrade, Serbia*

**16.00 – 16.15 Construction of Symmetry-adapted k.p Hamiltonians for semiconductor nanostructures**

Milan Jocić, Nenad Vukmirović

*Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade,  
Serbia*

**16.15 – 16.30 Application of nanomaterials in mechanical engineering**

Dorđe Jovanović<sup>1</sup>, Mladen Krstić<sup>2</sup>, Branislav Milenković<sup>3</sup>

*<sup>1</sup>Mathematical institute of SASA, Kneza Mihaila 36, 11000, Belgrade, Department of  
Computer Science, <sup>2</sup>Faculty of Mechanical and Civil Engineering, Dositejeva 19, 36000,  
Kraljevo, Department of Mechanical Engineering, Faculty of Applied Science, Dušana  
Popovića 22a, 18000, Niš, Department of Mechanical Engineering*

**16.30 – 16.45 Numerical study of coupled heat and moisture transfer in a finite wall:  
effect of wall material on transfer properties**

Zahreddine Hafsi

*Laboratory of Applied Fluids Mechanics Process and Environment Engineering, National  
Engineering School of Sfax, University of Sfax, Sfax 3038, Tunisia*



**Friday, December 3, 2021**

**09.00 – 10.30 10<sup>th</sup> Session – Materials for High-technology Application I**  
**Chairpersons: Dr. Dragana Jugović and Dr. Milica Vasić**

**09.00 – 09.15 Simply prepared Mg-V-O as potential cathode material for rechargeable aqueous magnesium ion batteries**

Milica M. Vasić<sup>1</sup>, Miloš Milović<sup>2</sup>, Danica Bajuk Bogdanović<sup>1</sup>, Milica Vujković<sup>1</sup>

<sup>1</sup>University of Belgrade - Faculty of Physical Chemistry, Belgrade, Serbia, <sup>2</sup>Institute of Technical Sciences of SASA, Belgrade, Serbia

**09.15 – 09.30 Layered CaV<sub>2</sub>O<sub>6</sub> as promising electrode material for multivalent storage**

Tamara Petrović<sup>1</sup>, Miloš Milović<sup>2</sup>, Danica Bajuk-Bogdanović<sup>1</sup>, Milica Vujković<sup>1</sup>

<sup>1</sup>Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, <sup>2</sup>Institute of Technical Sciences of SASA, Belgrade, Serbia

**09.30 – 09.45 Wearable Graphene Sensor for Pulse Measurement**

Teodora Vićentić<sup>1</sup>, Milena Rašljić Rafajilović<sup>1</sup>, Bojana Koteska<sup>2</sup>, Ana Madevska Bogdanova<sup>2</sup>, Igor Pašti<sup>3</sup> and Marko Spasenović<sup>1</sup>

<sup>1</sup>Center for Microelectronic Technologies, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Serbia, <sup>2</sup>Faculty of Computer Science and Engineering, "Ss. Cyril and Methodius" University of Skopje, North Macedonia, <sup>3</sup>Faculty of Physical Chemistry, University of Belgrade, Serbia

**09.45 – 10.00 Oxygen sensor based on mechanochemically treated metal oxide semiconducting TiO<sub>2</sub>-CeO<sub>2</sub> mixture**

Jelena N. Stevanović<sup>1</sup>, Srđan Petrović<sup>1</sup>, Dana Vasiljević-Radović<sup>1</sup>, Katarina Cvetanović<sup>1</sup>, Nenad Tadić<sup>2</sup>, Lazar Rakočević<sup>3</sup>, Milija Sarajlić<sup>1</sup>

<sup>1</sup>Institute of Chemistry, Technology and Metallurgy, Njegoševa 12, University of Belgrade, Belgrade, <sup>2</sup>Faculty of Physics, Cara Dušana 13, University of Belgrade, Belgrade, <sup>3</sup>Vinča Institute of Nuclear Science, Mike Petrovića Street 12-14, University of Belgrade, Belgrade

**10.00 – 10.15 Improving the electrocatalytic activity of nickel for HER in alkaline media by galvanic exchange with rhodium**

Lazar Bijelić, Aleksandar Jovanović, Igor Pašti

University of Belgrade – Faculty of Physical Chemistry, Belgrade, Serbia

**10.15 – 10.30 Hydrogen evolution on graphene supported PtAu nanoparticles**

Lazar Rakočević<sup>1</sup>, Ivana Stojković-Simatović<sup>2</sup>, Aleksandar Maksić<sup>1</sup>, Vladimir Rajić<sup>1</sup>, Svetlana Štrbac<sup>3</sup>, Irina Srejić<sup>1</sup>

<sup>1</sup>INN Vinca, Laboratory of Atomic Physics, University of Belgrade, Serbia, Mike Alasa 12-14, 11001 Belgrade, Serbia, <sup>2</sup>Faculty of Physical Chemistry, University of Belgrade, Serbia,

*Studentski trg 12-16, 11158 Beograd, Serbia, <sup>3</sup>Institute of Chemistry, Technology and Metallurgy, Department of Electrochemistry, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia*

## **10.30 – 10.45 Break**

## **10.45 – 12.15 11<sup>th</sup> Session – Materials for High-technology Application II Chairpersons: Dr. Zoran Jovanović and Vladimir Terek**

### **10.45 – 11.00 Electrochemical deposition for advanced engineering of novel electrocatalytic interfaces**

Aleksandar Z. Jovanović<sup>1</sup>, Sanjin J. Gutić<sup>2</sup>, Lidija Rafailović<sup>3</sup>, Igor A. Pašti<sup>1</sup>

<sup>1</sup>University of Belgrade – Faculty of Physical Chemistry, Belgrade, Serbia, <sup>2</sup>University of Sarajevo, Faculty of Science, Department of Chemistry, Sarajevo, Bosnia and Herzegovina, <sup>3</sup>CEST, Centre of Electrochemical Surface Technology, Wr. Neustadt, Austria

### **11.00 – 11.15 Effect of different cobalt loadings on the electrochemical performance of aluminum pillared clay-supported cobalt towards glucose oxidation**

Biljana Milovanović, Tihana Mudrinić, Sanja Marinović, Marija Ajduković, Aleksandra Milutinović-Nikolić, Predrag Banković

University of Belgrade - Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia, Department of Catalysis and Chemical Engineering, Njegoševa 12, Belgrade, Serbia

### **11.15 – 11.30 Synthesis and characterization of new dysprosium doped phosphate-tungsten bronze**

Tijana Maksimović<sup>1</sup>, Jelena Maksimović<sup>2</sup>, Pavle Tančić<sup>3</sup>, Ljubinka Joksović<sup>1</sup>, Maja Pagnacco<sup>4</sup>, Zoran Nedić<sup>2</sup>

<sup>1</sup>Faculty of Science, Department of Chemistry, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac, Serbia, <sup>2</sup>Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, 11001 Belgrade, Serbia, <sup>3</sup>Geological Survey of Serbia, Rovinjska 12, 11000 Belgrade, Serbia, <sup>4</sup>Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia

### **11.30 – 11.45 Novel PAN-based Air Filters for Potential Applications in Industrial Air Filtering and Facemask Production**

Mihailo Mirković<sup>1</sup>, Dušica Stojanović<sup>1</sup>, Daniel Mijailović<sup>2</sup>, Nemanja Barać<sup>2</sup>, Đorđe Janačković<sup>1</sup>, Petar Uskoković<sup>1</sup>

<sup>1</sup>University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia, <sup>2</sup>Innovation Center of Faculty of Technology and Metallurgy in Belgrade Ltd., Karnegijeva 4, 11120 Belgrade, Serbia

**11.45 – 12.00 High temperature tribological testings of TiAlN coating**

Vladimir Terek<sup>1</sup>, Lazar Kovačević<sup>1</sup>, Aleksandar Miletić<sup>2</sup>, Branko Škorić<sup>1</sup>, Aljaž Drnovšek<sup>3</sup>, Zoran Bobić<sup>1</sup>, Pal Terek<sup>1</sup>

<sup>1</sup>University of Novi Sad, Faculty of Technical Sciences, Department of Production Engineering, Novi Sad, Serbia, <sup>2</sup>Polytechnique Montreal, Department of Engineering Physics, Quebec, Canada, <sup>3</sup>Jožef Stefan Institute, Department of Thin Films and Surfaces Ljubljana, Slovenia

**12.00 – 12.15 Effects of corrosion on NiTi caused by fluoride and chloride media in non-accelerated corrosion tests**

Zoran Bobić<sup>1</sup>, Bojan Petrović<sup>2</sup>, Sanja Kojić<sup>1</sup>, Vladimir Terek<sup>1</sup>, Lazar Kovačević<sup>1</sup>, Goran Stojanović<sup>1</sup>, Branko Škorić<sup>1</sup>, Pal Terek<sup>1</sup>

<sup>1</sup>University of Novi Sad, Faculty of Technical Sciences, Department of production Engineering, Novi Sad, Serbia, <sup>2</sup>University of Novi Sad, Faculty of Medicine, Novi Sad, Serbia

**12.15 – 13.15 Lunch break**

**13.15 – 14.45 12<sup>th</sup> Session – Materials for High-technology Application III  
Chairpersons: Prof. Dr. Ljiljana Damjanović-Vasilić and S. Djurdjić Mijin**

**13.15 – 13.30 Raman Spectroscopy of Quasi-two-dimensional transition metal trihalides**  
S. Djurdjić Mijin<sup>1</sup>, AM Milinda Abeykoon<sup>2</sup>, A. Solajić<sup>1</sup>, A. Milosavljević<sup>1</sup>, J. Pešić<sup>1</sup>, M. Šćepanović<sup>1</sup>, Y. Liu<sup>3</sup>, A. Baum<sup>4,5</sup>, C. Petrović<sup>3</sup>, N. Lazarević<sup>1</sup>, Z. V Popović<sup>1,6</sup>

<sup>1</sup>Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia, <sup>2</sup>National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, New York 11973, <sup>3</sup>Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973-5000, United States, <sup>4</sup>Walther Meissner Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany, <sup>5</sup>Fakultät für Physik E23, Technische Universität München, 85748 Garching, Germany, <sup>6</sup>Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000 Belgrade, Serbia

**13.30 – 13.45 Finishing of polyamide fabric with some boron compounds**

Milena Nikodijević, Čedomir Dimić, Ivana Petrović, Dragan Đorđević  
Faculty of Technology, University of Niš

**13.45 – 14.00 Zeolite-containing photocatalysts immobilized on aluminum support by plasma electrolytic oxidation**

Kristina Mojsilović<sup>1</sup>, Nikola Božović<sup>1,2</sup>, Srna Stojanović<sup>3</sup>, Ljiljana Damjanović-Vasilić<sup>3</sup>, Maria Serdechnova<sup>4</sup>, Carsten Blawert<sup>4</sup>, Mikhail L. Zheludkevich<sup>4,5</sup>, Stevan Stojadinović<sup>1</sup>, Rastko Vasilić<sup>1</sup>

<sup>1</sup>Faculty of Physics, University Of Belgrade, Studentski trg 12-16, Belgrade 11000, Serbia,

<sup>2</sup>Directorate of Measures and Precious Metals, Mike Alasa 14, Belgrade 11000, Serbia,

<sup>3</sup>Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, Belgrade

11000, Serbia, <sup>4</sup>Institute of Surface Science, Hemholtz-Zentrum Hereon, Max-Planck-Straße

1, Geesthacht 21502, Germany, <sup>5</sup>Institute of Materials Science, Faculty of Engineering, Kiel University, Kaiserstraße 2, Kiel 24143, Germany

#### **14.00 – 14.15 Obtaining of healthcare textiles based on viscose fabric with improved sorption properties**

Mateja Korica<sup>1</sup>, Zdenka Peršin<sup>2</sup>, Lidija Fras-Zemljič<sup>2</sup>, Mirjana Kostić<sup>3</sup>

<sup>1</sup>Innovation Center of Faculty of Technology and Metallurgy, University of Belgrade, Serbia,

<sup>2</sup>Institute of Engineering Materials and Design, Faculty of Mechanical Engineering, University of Maribor, Slovenia, <sup>3</sup>Faculty of Technology and Metallurgy, University of Belgrade, Serbia

#### **14.15 – 14.30 Lattice dynamics and magnetism in Fe<sub>3-x</sub>GeTe<sub>2</sub>**

Ana Milosavljević<sup>1</sup>, Andrijana Šolajić<sup>1</sup>, Sanja Đurđić Mijin<sup>1</sup>, Jelena Pešić<sup>1</sup>, Bojana Višić<sup>1</sup>, Yu Liu<sup>2</sup>, Cedimir Petrović<sup>2</sup>, Zoran V. Popović<sup>1,3</sup>, Nenad Lazarević<sup>1</sup>

<sup>1</sup>Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade,

Serbia, <sup>2</sup>Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973-5000, USA, <sup>3</sup>Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000 Belgrade, Serbia

#### **14.30 – 14.45 Design of a pump for shipping crude oil from an oil terminal in Cameroon**

Lotin Thierry, Bella Marie

University of Douala, Faculty of sciences P.O. Box 245 Douala, Cameroon

#### **14.45 – 15.00 Break**

#### **15.00 – 16.45 13<sup>th</sup> Session – New Synthesis and Processing Methods and Materials for New Generation Solar Cells**

**Chairpersons: Prof. Dr. Ivana Stojković Simatović and Jelena Mitrić**

#### **15.00 – 15.15 Application of supercritical carbon dioxide for making perovskite photodiode**

Milica Stefanović<sup>1</sup>, Rada Petrović<sup>2</sup>, Ivana Lukić<sup>2</sup>, Jelena Vujančević<sup>3</sup>, Đorđe Janačković<sup>2</sup>

<sup>1</sup>University of Belgrade, Innovation Center of Faculty of Technology and Metallurgy,

Belgrade, Serbia, <sup>2</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>3</sup>Institute of Technical Sciences of SASA, Belgrade, Serbia

#### **15.15 – 15.30 Optimisation of materials for enhancement of efficiency of Dye Sensitized Solar Cells**

Evgenija Milinković<sup>1</sup>, Katarina Cvetanović<sup>1</sup>, Dana Vasiljević-Radović<sup>1</sup> and Dragomir Stanisavljev<sup>2</sup>

<sup>1</sup>Centre of Microelectronic Technologies, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoseva 12, 11060 Belgrade, Serbia, <sup>2</sup>Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, 11060 Belgrade, Serbia

**15.30 – 15.45 Investigation of photo(electro)catalytic efficiency of BaTi<sub>1-x</sub>Sn<sub>x</sub>, ZnO and ZnO@BaTi<sub>1-x</sub>Sn<sub>x</sub> (x = 0, 0.05, 0.10) powders**

Katarina Aleksić<sup>1</sup>, Ivan Supić<sup>2</sup>, Ivana Stojković Simatović<sup>2</sup>, Ana Stanković<sup>1</sup>, Smilja Marković<sup>1</sup>

<sup>1</sup>Institute of Technical Sciences of SASA, Belgrade, Serbia, <sup>2</sup>Faculty of Physical Chemistry, University of Belgrade, Serbia

**15.45 – 16.00 Thin film nanocomposites based on polyaniline and silver nanowires for optoelectronic applications**

Jovan Lukić, Vuk V. Radmilović

Faculty of Technology and Metallurgy, University of Belgrade, Serbia

**16.00 – 16.15 Surface phonons in YVO<sub>4</sub>:Eu<sup>3+</sup> nanopowders**

J. Mitrić<sup>1</sup>, N. Paunović<sup>1</sup>, M. Mitrić<sup>3</sup>, J. Ćirković<sup>2</sup>, M. Gilić<sup>1</sup>, M. Romčević<sup>1</sup> and N. Romčević<sup>1</sup>

<sup>1</sup>Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia,

<sup>2</sup>Institute for Multidisciplinary Research, University of Belgrade, Kneza Višeslava 1a, 11030 Belgrade, Serbia, <sup>3</sup>Institute Vinča, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

**16.15 – 16.30 Hydrothermal synthesis of hydroxyapatite on calcium-enriched natural and synthetic zeolite as a carrier**

Katarina Sokić<sup>1</sup>, Đorđe Veljović<sup>1</sup>, Jelena Dikić<sup>2</sup>, Jovica Stojanović<sup>3</sup>, Danijela Smiljanić<sup>3</sup>, Sanja Jevtić<sup>1</sup>

<sup>1</sup>Faculty of Technology and Metallurgy, University of Belgrade, Serbia, <sup>2</sup>Innovation centre of the Faculty of Technology and Metallurgy, University of Belgrade, Serbia, <sup>3</sup>Institute for Technology of Nuclear and Other Mineral Raw Materials, University of Belgrade, Serbia

**16.30 – 16.45 Synthesis of linear and star-shaped oligoimides by high-temperature catalytic polycondensation in a benzoic acid melt according to the Bn + AB scheme**

A.E. Soldatova<sup>1</sup>, A.Ya. Tsegelskaya<sup>1</sup>, I. G. Abramov<sup>2</sup>, A. Kh. Shakhnes<sup>3</sup>, O.V. Serushkina<sup>3</sup>, A. Herberg<sup>4</sup>, A.A. Kuznetsov<sup>1</sup>

<sup>1</sup>Enikolopov Institute of Synthetic Polymeric Materials, Moscow, Russia, <sup>2</sup>Yaroslavl State Technical University, Yaroslavl, Russia, <sup>3</sup>Zelinsky Institute of Organic Chemistry, Moscow, Russia, <sup>4</sup>Paderborn University, Paderborn, Germany

**16.50 Closing Ceremony**

1-1

### **Synthesis and characterization of the pH-sensitive saccharide-based polyurethane hydrogels**

Marija Kostić

*Faculty of Technology Novi Sad, University of Novi Sad, Novi Sad, Serbia*

Polymer hydrogels are widely used in medicine and pharmacy due to their biocompatibility and hydrophilicity. They are similar to living tissue and have wide application, for biosensors, separation membranes, artificial muscles, systems for controlled release of drugs, for the extraction of heavy metals and wastewater treatment. They change properties with changes in their environment, which is why hydrogels are called "intelligent" materials. The influence of the pH value of the environment for physiological, biological and chemical systems is especially important. Biodegradable polyurethanes can be the basis for drug delivery systems that are sensitive to external changes. One of the advantages of polyurethane is the possibility of achieving a different chemical structure by varying the stoichiometric parameters of the synthesis or starting materials. In this study pH-sensitive polyurethane hydrogels with a different polyol components (poly(ethylene glycol) 400/poly(propylene glycol) 2000/poly(ethylene glycol)-block-poly(propylene glycol)-block-poly(ethylene glycol) 1100), saccharides as crosslinkers (melibiose/raffinose/starch) and  $\alpha$ -hydroxy carboxylic acids as chain extenders (dimethylol propionic acid/lactic acid) were synthesized. Structural characterization of the synthesized polyurethane hydrogels was performed using Fourier transform infrared spectroscopy (FTIR), which showed that the polyurethane synthesis reaction was achieved with successful crosslinking with saccharides. Despite the change of starting components, FTIR spectra for all investigated samples are almost identical. The degree of swelling of the hydrogels was observed at 25 °C in solutions of pH values 4.5 and 7.4. The synthesized samples showed a higher degree of swelling at pH value 7.4. Polysaccharide starch as a crosslinker leads to a lower degree of swelling at pH - 7.4 (PPG2000SD - 3.32%) than the disaccharide melibiose (PPG2000MD - 11.44%). The effects of variable parameters on the phase transitions of polyurethane hydrogels were investigated by differential scanning calorimetry (DSC). The change in the length of the polyol chain led to differences in the value of  $T_{gss}$ , whereas in the samples with shorter polyol chains the  $T_{gss}$  is higher compared to the samples with longer polyol chains. The results showed that by varying the saccharide as a crosslinker, the acid chain extender and the chain length of the polyols, the stated properties of polyurethane hydrogels can be influenced.

1-2

**Antiradical activity of graphene quantum dots enriched albumin hydrogel:  
An EPR study**

Đura Nakarada<sup>1</sup>, Vladimir Trajković<sup>2</sup>, Miloš Mojović<sup>1</sup>

<sup>1</sup>*University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia*

<sup>2</sup>*University of Belgrade, Faculty of Medicine, Belgrade, Serbia*

Graphene quantum dots (GQD) are single to multilayer carbon-based nanoparticles. They possess high chemical and physical stability, high biocompatibility, low toxicity, and are easily dispersible in water. These properties make them a novel material for the therapeutical application. Due to their antiradical scavenging activity, GQD are considered to be a promising material in terms of inhibiting oxidative damage caused by the elevated level of free radicals. Serum albumin is the primary carrier of various solutes in blood plasma and is commonly used in solubilizing therapeutics. It is suitable for the production of biological hydrogels which are biocompatible and have medical significance as efficient site-located drug delivery systems. This research aims to examine the antiradical activity of GQD incorporated into the albumin hydrogel towards  $\cdot\text{OH}$  radicals and their ability to induce prolonged scavenging effects. Since  $\cdot\text{OH}$  radicals are short-lived species, the electron paramagnetic resonance (EPR) spin-trapping technique (and spin-trap DEPMPO) has been used for their detection. Gellation of bovine serum albumin (BSA) solution containing GQD has been thermally induced. The obtained gel has been introduced into the Fenton reaction ( $\cdot\text{OH}$  radicals generator) system containing the spin-trap and gently stirred. To estimate the antiradical effect arising from GQD, control experiments were performed using BSA hydrogel without GQD as well as by replacing BSA hydrogel with water. The obtained results indicate that BSA itself possesses certain antiradical activity, since it eliminated 19.84 % of  $\cdot\text{OH}$  radicals from the system. However, the most significant elimination of  $\cdot\text{OH}$  radicals has been observed in the system containing GQD (99.86 %), where 80.02 % of  $\cdot\text{OH}$  radicals have been eliminated entirely by GQD. Our results show the significant potential of albumin hydrogels as GQD carriers, as well as the compelling anti-hydroxyl radical scavenging efficiency of the GQD. These results give a promising perspective in the light of the synergical effect of GQD albumin hydrogels as site-located radical scavengers.

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1-3

**Characteristics of thin films of biological substances deposited on  
polyethylene terephthalate (PET) in terms of biomedical applications**

K. Szafran<sup>1</sup>, M. Jurak<sup>1</sup>, R. Mroczka<sup>2</sup>, A.E. Wiącek<sup>1</sup>

<sup>1</sup>*Department of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of Chemistry,  
Maria Curie-Skłodowska University, Lublin, POLAND,* <sup>2</sup>*Laboratory of X-Ray Optics, Centre  
for Interdisciplinary Research, Faculty of Science and Health, The John Paul II Catholic  
University of Lublin, Poland*

Polyethylene terephthalate (PET) is a polymer used in medicine for the production of blood vessel prostheses, organs (e.g. artificial hearts) or temporary tendons. However, the hydrophobic nature and the inertness of its surface result in poor compatibility with human tissues leading to rejection of the implant. Therefore, in order to improve the compatibility of the polymer, thin films of biological substances are deposited on its surface. A phospholipid - 1,2-dioleoyl-*sn*-glycero-3-phosphocholine (DOPC), having a double bond in each hydrocarbon chain, is the main building component of most biomembranes. As a result, it can be a link between the foreign body (implant surface) and the biological environment, increasing the likelihood of a positive response from the body, and at the same time facilitating the introduction and subsequent release of an active substance such as cyclosporin A (CsA). It is a strong immunosuppressive drug widely used in medicine, among others to prevent rejection of a transplant/implant. However, the administration of this drug has many side effects due to the generation of reactive oxygen species. Their presence causes lipid peroxidation leading to damage to the integrity of the cell membrane. In order to reduce these undesirable effects, it is necessary to use an antioxidant. One of them is lauryl gallate (LG), which, as an active derivative of gallic acid, can eliminate free radicals, protecting the phospholipids against peroxidation.

The aim of the study was to investigate the properties of Langmuir-Blodgett layers containing biological and bioactive substances using secondary ion mass spectrometry with a time-of-flight analyzer (TOF-SIMS), atomic force microscopy (AFM) and wettability measurements along with estimation of surface free energy and its components.

Our findings indicate for the increase in surface polarity with LG molar fraction which results from specific interactions between components within the layer and the exposure of groups capable of interacting with liquids of various nature. Controlling of the hydrophilic-hydrophobic properties depending on the composition of the films may contribute to the emergence of the system with the highest biocompatibility.

1-4

**Additive-free resveratrol micro- and nanoparticles and assessment of their toxicity**

Nina Tomić<sup>1</sup>, Maja Kuzmanović<sup>1</sup>, Dragana Mitić Ćulafić<sup>2</sup>, Magdalena M. Stevanović<sup>1</sup>

<sup>1</sup>*Institute of Technical Sciences of SASA, Knez Mihailova 35/IV 11000 Belgrade, Serbia*

<sup>2</sup>*Department of Microbiology, University of Belgrade - Faculty of Biology, Studentski trg 16, Belgrade, Serbia*

Resveratrol, polyphenol from stilbene family, has demonstrated beneficial effects on human health in numerous studies. Among these effects are cardioprotective, anti-cancer, neuroprotective, antimicrobial and other. *In vivo*, application of this phytochemical often lacks significant results. This is mainly because of its poor bioavailability, caused by low water solubility, sensitivity to light, oxygen and pH change, and high reactivity. Micro- and nanoformulations of resveratrol have been described to highly improve bioavailability. However, there are limitations to this approach, such as demanding synthesis process, necessity of expensive or toxic chemicals, or poor loading capacity. We have used a simple physicochemical solvent-non solvent method to synthesise additive-free, stable and uniform elongated resveratrol micro- and nanoparticles (RES-particles). The drying conditions were varied to examine their influence on the morphological characteristics of resveratrol particles. Differential effects of drying at ambient, low, and elevated temperature as well as effects of centrifugation and stability of RES-particle suspension during the time were documented. RES-particles were characterized by X-ray diffraction (XRD), differential scanning calorimetry (DSC), ultraviolet-visible (UV-Vis) spectrophotometry, Fourier transform infrared spectroscopy (FTIR) and optical microscopy. Biocompatibility of RES-particles was preliminary assessed through MTT toxicity assay.

1-5

**The use of Langmuir's technique to assess  
the antibacterial properties of chemical substances**

Agata Ładniak<sup>1</sup>, Małgorzata Jurak<sup>1</sup>, Marta Palusińska-Szys<sup>2</sup>,  
Klaudia Woźniak<sup>1</sup>, Kacper Przykaza<sup>1</sup>, Agnieszka Ewa Wiącek<sup>1</sup>

<sup>1</sup>*Institute of Chemical Sciences, Department of Interfacial Phenomena, Faculty of Chemistry,  
Maria Curie-Skłodowska University, M. Curie-Skłodowska Sq. 3, 20-031 Lublin, Poland*

<sup>2</sup>*Institute of Biological Sciences, Department of Genetics and Microbiology, Faculty of  
Biology and Biotechnology, Maria Curie-Skłodowska University, Akademicka 19, 20-033  
Lublin, Poland*

Langmuir's technique is powerful tool to assessment the influence of various substances on biological membranes. Although this method enables the characterization of only monomolecular films at the interface, there is a strong correlation between the properties (pressure, surface area per lipid molecule, phase transition, compressibility) of mono- and bilayers prepared from cell membrane components, at surface pressures of 30-35mN/m. Owing to this, it is possible to predict interactions with high probability at the level of living organisms. Knowledge about the organization of monolayers and their interactions with the components of the support and the possibility of their control at the molecular level determine the potential usefulness of the obtained bioproducts and enable the development of a wide range of science and technology.

The aim of the study was to verify the effect of (inter alia) biopolymers such as chitosan – polycationic in nature, and hyaluronic acid which is a polyanion on model biological membranes, formed of biological material, i.e. lipids extract isolated from two kinds of bacteria: Gram-negative *Escherichia coli* and Gram-positive *Staphylococcus aureus*. This allowed to confirm the assumption that the mechanism of the antibacterial action of these compounds and their mixtures is based on disturbances in the cell membrane of microorganisms.

The obtained results clearly showed that these biopolymers affect the structure of bacterial membranes. They induced various changes in membrane structure, ultimately hindering the formation of a compact, rigid film of both *E. coli* and *S. aureus*.

2-1

**Development of a physiologically relevant 3D *in vitro* model for osteosarcoma cell cultivation comprising alginate composite scaffolds and a perfusion bioreactor system**

Ivana Banićević<sup>1</sup>, Mia Radonjić<sup>1</sup>, Marija Pavlović<sup>1</sup>, Milena Milivojević<sup>2</sup>,  
Milena Stevanović<sup>2,3,4</sup>, Jasmina Stojkowska<sup>1,5</sup>, Bojana Obradović<sup>1</sup>

<sup>1</sup>Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

<sup>2</sup>Institute of Molecular Genetics and Genetic Engineering, University of Belgrade, Belgrade, Serbia, <sup>3</sup>Faculty of Biology, University of Belgrade, Belgrade, Serbia, <sup>4</sup>Serbian Academy of Sciences and Arts, Belgrade, Serbia, <sup>5</sup>InnovationCenter of the Faculty of Technology and Metallurgy, Belgrade, Serbia

Osteosarcoma is the most common type of bone cancer, which affects both children and adults. Treatment of osteosarcoma exhibits slow progress due to inadequacy of both *in vivo* animal models and 2D *in vitro* models regularly used for antitumor drug testing. Our approach is to create a physiologically relevant 3D *in vitro* model for osteosarcoma cell cultivation, which has the potential to overcome inherent weaknesses of 2D *in vitro* and animal models. In order to imitate native osteosarcoma microenvironment, macroporous alginate scaffolds with incorporated hydroxyapatite/ $\beta$ -tricalcium phosphate (HAp/ $\beta$ -TCP) powder were produced with two compositions: 1 wt% alginate, 1 wt% powder and 2 wt.% alginate, 2 wt% powder. Bioactivity and stability of the scaffolds were investigated under biomimetic conditions of continuous flow of the culture medium in perfusion bioreactor at the superficial medium velocity of 400  $\mu\text{m/s}$ , which was reported in literature to be beneficial for osteogenesis. Scaffolds with the higher alginate concentration was shown to be more stable in the culture medium, since the scaffolds with the lower alginate concentration disintegrated after 5-7 days under flow conditions. Biocompatibility of the obtained scaffolds was investigated in short-term cultivation studies of murine osteosarcoma cells K7M2-wt seeded onto the scaffolds. The scaffolds were cultivated in perfusion bioreactors at the superficial flow velocity of 15  $\mu\text{m/s}$ , while static cultures served as a control. After cultivation, osteosarcoma cells remained adhered to the scaffold surface, expressed metabolic activity and retained their initial proliferation ability while the flow was shown to positively affect the cultivated cells.

2-2

**Electrochemical composite bioceramic coatings based on hydroxyapatite, chitosan and polyvinyl alcohol loaded with gentamicin**

Nevena Jaćimović<sup>1</sup>, Marija Došić<sup>2</sup>, Ana Janković<sup>1</sup>, Vesna Mišković – Stanković<sup>1</sup>

<sup>1</sup>*Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, Belgrade, Serbia,* <sup>2</sup>*Institute for Technology of Nuclear and Other Mineral Raw Materials, Bulevar Franš d'Eperea 86, Belgrade, Serbia*

Composite bioceramic coatings have been attracting increasing attention of the scientific public in recent decades due to the good potential of their use for medical purposes. The main goal of this scientific research is to show the characterization of the obtained hydroxyapatite (HAP), chitosan (CS) and polyvinyl alcohol (PVA) bioceramic composite coatings loaded with gentamicin (Gent), on titanium (Ti) substrate using the single-step electrophoretic deposition process. Titanium, traditionally used for the purpose of replacing parts of damaged bone tissue, has shown good mechanical properties and biocompatibility through many years of orthopedic practice. Hydroxyapatite provided the HAP/CS/PVA/Gent composite coating with osteoinductivity, while the presence of chitosan and polyvinyl alcohol contributed to its adhesive and mild analgesic properties. The antibacterial agent gentamicin was added to the HAP/CS/PVA composite, which ensured its direct antibacterial effect at the implantation site. The coatings were deposited using the cathodic electrophoretic deposition process, with the Ti plate as the cathode, at a constant voltage of 7V, in the range of the deposition time from 5 to 12 min. To demonstrate the presumed bioactivity, HAP/CS/PVA/Gent coatings were immersed in simulated body fluid (SBF) at 37°C for periods of 7 and 14 days. Characterization of HAP/CS/PVA/Gent coatings after immersion was performed through employment of Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), and field emission scanning electron microscopy (SEM) techniques. Antibacterial activity was tested by agar diffusion method on two bacterial strains, *Escherichia coli* and *Staphylococcus aureus* with a positive response to both bacterial strains. The final conclusions of this research suggest a good potential for utilization of HAP/CS/PVA/Gent bioceramic composite coating, applied through electrophoretic deposition process on Ti substrate, for medical purposes in the replacement and healing of damaged bone tissue.

2-3

### **Optimization of Bioreactor Cultures of Glioblastoma Cells Immobilized in Alginate Microfibers**

Jelena Petrovic<sup>1,2</sup>, Mia Radonjic<sup>1,2</sup>, Jasmina Stojkovska<sup>1,2</sup>, Bojana Obradovic<sup>1</sup>

<sup>1</sup>*Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia,*

<sup>2</sup>*Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia*

Glioblastoma is the most common and aggressive malignant brain tumor in adults. Existing treatment choices that include surgery, radiation and chemotherapy are not successful in long-term survival, while development of new anticancer drugs is being held back by the lack of adequate model systems for anticancer drug testing. Namely, in traditionally used two-dimensional (2D) monolayer cancer cell cultures the native cell morphology, polarity and interactions between both cells and cells and extracellular components are either changed or absent, while studies on animals often produce misleading results due to interspecies differences. Hence, there is a pressing need for new glioblastoma model systems that provide more in vivo-like environment for investigation and development of new anticancer drugs. The aim of this work was to develop a biomimetic 3D environment for cultivation of glioblastoma cells based on alginate microfibers as cell carriers and perfusion bioreactors. Previous studies have shown that static cultures of cervical cancer cells SiHa immobilized in alginate microfibers may be diffusion limited while perfusion, which enhanced mass transport, has induced negative effects on human embryonic teratocarcinoma cells NTERA-2 in superficial zones of alginate microbeads by hydrodynamic shear stresses. Thus, in the present study, the specific focus was on optimization of cell concentration within microfibers and regimes of cultivation to achieve beneficial effects of fluid flow in perfusion bioreactors. A series of experiments were conducted in which the concentration of rat glioma cells C6 was varied between  $2$  and  $8 \times 10^6$  cell  $\text{cm}^{-3}$  at several flowrates and regimes of static and perfusion culture periods. Mixed results were obtained implying that efficient mass transport has a higher effect in microfiber cultures at lower cell concentrations (*i.e.*  $\sim 2 \times 10^6$  cell  $\text{cm}^{-3}$ ). In specific, medium flow at the superficial velocity of  $100 \mu\text{m s}^{-1}$  induced considerable cell proliferation as compared to control static cultures, which maintained the initial cell numbers. Mathematical modelling indicated that the convective transport of substances with low diffusion coefficients ( $\sim 10^{-19} \text{ m}^2 \text{ s}^{-1}$ ) may have induced the observed positive effects. Still, exact relations of cultivation conditions and cell responses in terms of viability, proliferation and metabolic activity should be further investigated.

2-4

### **Laser induced periodic surface structures on Ti thin films by ultrafast laser irradiation**

Nevena Božinović<sup>1</sup>, Vladimir Rajić<sup>1</sup>, Danilo Kisić<sup>1</sup>,  
Dragana Tošić<sup>1</sup>, Dubravka Milovanović<sup>2</sup>, Suzana Petrović<sup>1</sup>,

<sup>1</sup>*Department of Atomic Physics, Vinča Institute of Nuclear Sciences, National Institute of the  
Republic of Serbia, P.O. Box 522, 11001 Belgrade, University of Belgrade, Serbia;*

<sup>2</sup>*University of Belgrade, Institute of General and Physical Chemistry, Studentski trg 12/V,  
11158 Belgrade, Serbia*

In this study, design of surface patterning with the co- existence of micro- and nanoscale features by pico- and femtosecond laser processing is investigated toward to improve the arrayed surface structures on Ti multilayer thin films. Composite structures consist of two layers of Ti and subsurface distributed Cu and Zr layers (thickness of 10 nm) were deposited by ion sputtering on Si substrate to the total thickness of 300 nm. The changes of the composition, surface morphology and wetting properties after laser modification were monitored by scanning electron microscopy (SEM-EDS), atomic force microscopy (AFM), optical profilometry and wetting measurements. It was found that picosecond laser irradiation can induced melting of material with formation wrinkled periodic structures at the edges of the laser spots in both systems as a consequence of the hydrodynamic effects. Interesting result irradiated with both laser beams is that the formation periodic structures in form of ripples is slight pronounced in the sample with Zr as an ultra- thin subsurface layer. The results of EDS are reflected in the changes of component distribution between different periodic structures. In laser-induced periodic surface structure (LIPSS), a decrease in the content of thin film components (Ti, Zr, Cu) was observed, while the Si concentration increased, which indicates that material ablation occurred. AFM analysis confirmed increasing of the mean surface roughness almost 98 nm for both samples in the laser-written lines (after femtosecond irradiation), which was proven on 2D profiles by optical profilometry. Contact angle measurements indicated acceptable wettability of deionized water after laser processing, which makes these materials appropriate for exploring biological response, especially due to presence biocompatible non-toxic elements (Zr and Cu).

2-5

**Omitting mischmetal and zirconium as a next step  
in the development of biodegradable magnesium implants**

Maria Zemkova<sup>1</sup>, Peter Minarik<sup>1</sup>, Eva Jablonska<sup>2</sup>, Jozef Vesely<sup>1</sup>, Jan Bohlen<sup>3</sup>, Robert Kral<sup>1</sup>

<sup>1</sup>Charles University, Ke Karlovu 5, 121 16 Prague, Czech Republic, <sup>2</sup>University of Chemistry and Technology, Technická 5, 166 28 Prague, Czech Republic, <sup>3</sup>Helmholtz-Zentrum Geesthacht, Magnesium Innovation Center, Max-Planck-Straße 1, 215 02 Geesthacht, Germany

The recent intensive development of the magnesium-based degradable implants showed that the Mg-Y-RE-Zr alloying system (WE-type) provides a satisfying degradation rate together with mechanical strength. Alloys from this system are often investigated in various *in vitro* and *in vivo* studies and already also in clinical trials. However, utilization of both mischmetal and zirconium in the WE-type alloys were originally driven by the industrial demand for magnesium alloys suitable for high-temperature applications. This study shows that omitting both of these elements does not compromise the appropriate biocompatibility and degradation rate of the Mg-3Y alloy. Loss of positive effect of mischmetal and zirconium on the mechanical strength can be compensated by a significant grain refinement via severe plastic deformation. Mg-3Y alloy processed by equal channel angular pressing, resulting in ultrafine-grained microstructure and weak crystallographic texture, exhibited compressive yield strength of 362(6) MPa and plastic deformation to fracture of 18(1)% with the same degradation rate in biologic media and cytotoxicity as the well-known Mg-Y-RE-Zr alloy. The results of this work unambiguously showed that utilization of mischmetal and zirconium is not necessary for the biodegradable applications of magnesium and can be easily avoided.



2-6

**Photo-activation of a dental composite from within  
using optical fibers – a holographic study**

Evgenije Novta<sup>1</sup>, Tijana Lainović<sup>1</sup>, Dušan Grujić<sup>2</sup>,  
Svetlana Savić-Šević<sup>2</sup>, Dejan Pantelić<sup>2</sup>, Larisa Blažić<sup>1,3</sup>

*University of Novi Sad, Faculty of Medicine, School of Dental Medicine, Novi Sad, Serbia*

*University of Belgrade, Institute of Physics, Belgrade, Serbia*

*Dental Clinic of Vojvodina, Novi Sad, Serbia*

The main limitation of light-activated dental resin-based composites (RBC) is polymerization shrinkage (PS) during polymer chain formation. This study aimed to examine the impact of a novel two-step photo-activation method of RBCs from within, using optical fibers, on PS. Tooth model deformation as a secondary manifestation of PS was measured in real-time using digital holographic interferometry (DHI).

Models with standardized tooth cavities (n=5) were mounted in aluminum blocks and fixed in the custom-made DHI set-up. The cavities were filled with a bulk-fill RBC. The proposed two-step curing was designed as follows: in the first step optical fibers connected to a commercial dental LED were inserted into the dental filling to cure the RBC from within; in the second step fibers were extracted, remaining voids were filled with the RBC, and final conventional curing was performed. Optical fibers with two different core diameters were examined (1 mm and 1.5 mm), forming two experimental groups. Conventional curing was used as a control. One-way ANOVA and post-hoc Dunnett's test were used to compare final deformation values between groups at  $\alpha=0.05$  level.

The results of Dunnett's test presented a statistically significant difference between the control group and both experimental groups ( $p=0.0$ ). The mean deformation value in the control group was 13.8  $\mu\text{m}$ , while in the 1 mm and 1.5 mm group it was 10.5  $\mu\text{m}$  and 8.6  $\mu\text{m}$ , respectively. The final deformation in the 1 mm and 1.5 mm groups was on average 24 % and 38 % lower, respectively, compared with the control group.

Within the limitations of this study, it can be concluded that the proposed photo-activation method influenced a significant decrease in PS compared to conventional curing. The utilization of 1.5 mm optical fibers was presented as more beneficial for PS reduction. Further examination is needed regarding the degree of monomer conversion and viscoelastic changes during polymerization

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3-1

### **Electrophoretic deposition vs. dip-coating of the bioceramic layers on Ti6Al4V scaffolds**

Marija Milivojević<sup>1</sup>, Željko Radovanović<sup>1</sup>, Suzana Dimitrijević<sup>2</sup>,

Miljana Popović<sup>2</sup>, Rada Petrović<sup>2</sup>, Đorđe Veljović<sup>2</sup>, Đorđe Janačković<sup>2</sup>

<sup>1</sup>*Innovation Center of Faculty of Technology and Metallurgy, Belgrade, Serbia,*

<sup>2</sup>*Faculty of Technology and Metallurgy University of Belgrade*

3D printed Ti6Al4V have been used in clinical practice to provide mechanical support for the regeneration of large bone defects. However, the bioinert surface of Ti6Al4V alloy needs to be improved. Coating with bioactive materials enables improvement of bioactivity and this strategy can also be employed to introduce antibacterial properties. A homogenous coating on a 3D printed scaffold presents a challenge as the macroporous architecture of the implant makes difficulties in standard coating procedures.

The aim of this study was to modify the surface of a 3D printed porous Ti6Al4V scaffold by coating it with bioactive glasses (BAG) and Ag-doped calcium hydroxyapatite (Ag-HAP), to provide bioactivity and antibacterial properties. Two standard coating techniques, electrophoretic deposition and dip-coating, were modified to provide homogenous and uniform coating inside the porous structure of the titanium sample. Heating microscopy analysis was employed to determine a melting point of BAG, in order to set up an annealing protocol for deposited BAG particles. The morphology and cross-sections of obtained coatings were analyzed using scanning electron microscopy (SEM), and the thickness and uniformity of the coatings obtained by the electrophoretic deposition and dip-coating were compared. Prolonged antibacterial properties of coated scaffolds against *E.coli* were evaluated. The bioactivity of the obtained coatings was examined in simulated body fluid (SBF).

In conclusion, modified electrophoretic deposition and dip-coating techniques made it possible to obtain uniform and homogenous bioceramic coating on 3D printed titanium scaffolds.

3-2

### **Dental inserts based on calcium hydroxyapatite: The influence of cation doping**

Tamara Matić<sup>1</sup>, Maja Ležaja Zebić<sup>2</sup>, Vesna Miletić<sup>3</sup>,  
Rada Petrović<sup>4</sup>, Đorđe Janačković<sup>4</sup>, Đorđe Veljović<sup>4</sup>

<sup>1</sup>University of Belgrade, Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>2</sup>University of Belgrade, School of Dental Medicine, Belgrade, Serbia,

<sup>3</sup>The University of Sydney, Faculty of Medicine and Health, Sydney Dental School, Surry Hills NSW, Australia, <sup>4</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

Large teeth restorations have a relatively short life span due to the polymerization shrinkage (PS) of the resin-based composites (RBCs) commonly used in restorative dentistry. In order to overcome this problem bioceramic inserts based on calcium hydroxyapatite (HAP), the main inorganic component of tooth structure, have been proposed as dentin substitutes. Biological apatite present in dentin has a variety of dopants in the structure such as Mg, Sr, Cu, which play an important role in the dentin formation and remineralization.

The application of cation doped HAP inserts could improve the biological response of the tissue, prolong its lifespan by reducing PS and simplify the clinical procedure. However, the presence of dopants leads to the lattice distortion, which influences solubility and mechanical properties of the hydroxyapatite based materials.

This study aimed to investigate the effects of single and bi- dopant calcium substitutions in hydroxyapatite structure on the phase composition and bonding ability of dental inserts with a commercially available restorative material. Hydroxyapatite nanopowders doped with Mg, Sr and Mg+Sr were obtained hydrothermally and pressed into compacts which were further sintered at 1200 °C. The restorative material used was Filtek Z\_250 composite applied with Single Bond Universal adhesive (SBU\_Z250). The bonding ability of inserts with SBU\_250 was tested using the Shear Bond Strength (SBS) test. The dopants were shown to have a great impact on the phase composition of thermally treated hydroxyapatite, thus on the bonding ability with SBU\_250.

3-3

### **Synthesis and antimicrobial properties of ZnO deposited on hydroxyapatite**

Marija Stevanović<sup>1</sup>, Rada Petrović<sup>2</sup>, Đorđe Veljović<sup>2</sup>,  
Suzana Dimitrijević<sup>2</sup>, Đorđe Janačković<sup>2</sup>

<sup>1</sup>*Inovacioni Centar Tehnološko-metalurškog fakulteta u Beogradu d.o.o.*, <sup>2</sup>*Tehnološko-metalurški fakultet Univerzitet u Beogradu*

Biological hydroxyapatite (HAP) presents an integral part of human bones and teeth, and thus has been intensively studied as a material for biomedical application. Synthetic HAP has good biocompatibility which makes it a suitable material for different applications in restorative and preventive dentistry. Dental caries and periodontal disease are the most prevalent oral diseases for which no perfectly regenerative solutions are available yet. The main reason for endodontic failure is the presence of some bacterial species inside the root canal system such as *Enterococcus (E.) faecalis*. Those bacteria are most resistant to disinfection agents, causing a persistent intra-radicular or extra-radicular infection. Due to excellent antimicrobial properties of zinc-oxide (ZnO) and biocompatibility of HAP, combination of ZnO deposited on hydroxyapatite particles seems to be promising materials for dental application. The goal of our work was to obtain antibacterial biomaterial by creating a material consisting of ZnO and HAP, optimizing the ZnO content and investigating its potential advantages in the dental application. The HAP was synthesized hydrothermally while ZnO was obtained by sonochemical method. The obtained powders were characterized through scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), and X-ray diffraction (XRD) techniques. The antimicrobial activity of the powder was evaluated against *Enterococcus (E.) faecalis*. The results showed a remarkable antimicrobial effect against one of the main dental pathogens, which makes the ZnO/HAP biocomposite a promising material for application in dental therapy.

3-4

**Processing of gelatine coated composite scaffolds based on magnesium and strontium doped hydroxyapatite and yttria-stabilised zirconium oxide**

Aleksa Galić<sup>1</sup>, Tamara Matić<sup>2</sup>, Nataša Obradović<sup>2</sup>, Đorđe Veljović<sup>1</sup>

<sup>1</sup>University of Belgrade, Faculty of Technology and Metallurgy, Department of Inorganic Chemical Technologies, Karnegijeva 4, 11000 Belgrade, Serbia, <sup>2</sup>Innovation Center of Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Belgrade, Serbia

Autologous and allogenic grafts are often referred to as the gold standard for bone tissue transplants, but possess drawbacks such as risk of immunological reaction and infection, limited bone bank capacity and pain for the patient, which is why synthetic transplants are a highly researched topic.

The goal of the research was to process and test the mechanical properties and bioactivity of the magnesium and strontium doped hydroxyapatite gelatine coated scaffolds and the impact of adding yttria-stabilized zirconium oxide for potential use in bone tissue engineering.

The doped hydroxyapatite powder was synthesized using the hydrothermal method and calcinated. The foam replica method was chosen for production of the scaffolds. Both sample groups, with and without the added zirconium-dioxide, were sintered in the range of 1400-1470 °C, and further coated in gelatine solution. Compressive strength was tested using a universal testing machine and bioactivity was inspected after 7 days in simulated body fluid. Element analysis was done using energy dispersive spectroscopy, X-ray diffraction analysis was done to determine the phase composition of the synthesized powder and sintered scaffolds. The morphology of the powder and microstructure of the scaffolds were analyzed using scanning electron microscopy.

Element analysis showed a Ca/P molar ratio of 1.31 and dopant fractions of Mg and Sr ions of 0.4 and 0.7 at%, respectively. The diffractogram of the calcined powder showed a biphasic system,  $\beta$ -TCP being the majority. Scaffolds withstood satisfactory forces up to 3 N and after soaking mechanical properties were certainly improved. A macroporous structure was achieved with the pores in both sample groups being interconnected and having the mean size of 250  $\mu\text{m}$ . The hydroxyapatite samples showed greater bioactivity than the composite samples.

Greater bioactivity and compressive strength of the doped hydroxyapatite scaffolds make them potential candidates for use in bone tissue engineering, while higher temperatures are needed for scaffolds with zirconia.

3-5

### **Dissolving and water absorption ability of spray-dried willow gentian extract**

Miloš Jovanović<sup>1</sup>, Nada Ćujić-Nikolić<sup>1</sup>, Zorica Drinić<sup>1</sup>,  
Teodora Janković<sup>1</sup>, Smilja Marković<sup>2</sup>, Katarina Šavikin<sup>1</sup>

<sup>1</sup>*Institute for Medicinal Plants Research “Dr. Josif Pančić”, Tadeuša Koščuška 1, 11000 Belgrade,* <sup>2</sup>*Institute of Technical Sciences of SASA, Knez Mihailova 35/IV, 11000 Belgrade*

Roots of the willow gentian (*Gentiana asclepiadea* L., Gentianaceae) are used in folk medicine to treat gastrointestinal diseases. Spray drying is the most commonly used technique for microencapsulation of plant extracts in the pharmaceutical, cosmetic and food industries. The choosing of suitable carriers is one of the critical points in the development of microencapsulated powder with the desired physicochemical properties. The extract of the willow gentian roots was spray-dried using different carriers (maltodextrin (MD) and whey protein (WP) at concentrations of 20, 40, and 60%; pectin (P), starch (S), and gelatin (G) at concentrations of 2.5, 5, and 7.5%). The aim of this study was to examine the ability of the obtained powder to dissolve and absorb water. For this purpose, the values of water solubility (WSI) and water absorption index (WAI) were determined. WSI is a measure of the powder degradation and dissolving in water, while WAI represents an indicator of water absorption ability. It is desirable that instant tea powders show high WSI and low WAI values. WSI values ranged from 71.15% (7.5% P) to 91.94% (7.5% G) indicating good powder disintegration properties. Concentration-dependent decrease in WSI values was observed for WP, P and S, while the opposite trend was observed in the case of MD. The carrier-free powder showed relatively low WAI value (13.32%). Powders with 20% MD and 5% S showed slightly lower WAI values (12.77 and 12.72%, respectively). On the other hand, powders with 5 and 7.5% P showed remarkably high WAI values of 91.59 and 91.49%, respectively. A concentration-dependent increase in WAI was observed in powders encapsulated with MD and WP. All encapsulated powders showed acceptable disintegration properties (high WSI), while in terms of water absorption (low WAI) powders with 20% MD and 5% S were the most suitable.

4-1

### **Hydrophobization, a method of monument protection**

Joanna Podkościelna, Konrad Terpiłowski

*Department of Interfacial Phenomena, Institute of Chemical Sciences,  
Faculty of Chemistry, Maria Curie Skłodowska University Lublin, Poland*

Rocks and ceramic materials have been used for construction purposes and as a material of art for centuries. The objects created over time are today valuable cultural monuments. According to Polish law, a monument is defined as "real estate or movable property, parts or complexes thereof, being a work of man or related to his activity and representing a bygone era or events whose preservation is in the public interest due to their historical, artistic or scientific value".

In the following work, in order to check the quality of coatings obtained with the use of impregnants available on the market, a test was carried out to assess the hydrophobic properties of the obtained coatings on various materials and their durability after exposure to weather conditions.

Coatings with the best hydrophobic properties were obtained by using agents based on organic solvents. Especially in the case of limestone rock, there is a clear difference in the values of the contact angles obtained with these agents compared with those based on water. Despite the better effects obtained with preparations based on organic solvents, the disadvantage of these agents is their toxicity and negative impact on the natural environment.

4-2

**Optimization of biodiesel production from waste cooking oil  
using waste-based CaO/zeolite catalyst**

Stefan Pavlović, Dalibor Marinković, Miroslav Stanković

*University of Belgrade, Institute of Chemistry, Technology, and Metallurgy-National  
Institute of Republic of Serbia, Njegoševa 12, 11000 Belgrade*

Lignite coal fly ash collected from Serbian thermal power plants was converted into value-added zeolite-like material using a Teflon-lined hydrothermal reactor in an alkali activation process at 150 °C for 24 h. The obtained material was used in the synthesis of zeolite-supported chicken eggshell calcium oxide catalyst for biodiesel synthesis from waste cooking oil using earlier established procedures. The study aimed to coupled optimization of catalyst synthesis parameters (CaO loading and calcination temperature) and biodiesel synthesis process (CaO concentration in the reaction mixture). The influence of calcination temperature in the catalyst activation stage was monitored by X-ray diffraction and FT-IR spectroscopy, whereas the reaction progress by the HPLC analysis. The analyzed calcination temperature range was within 450 °C and 950 °C, CaO loading in the range of 10 wt% - 50 wt%, whereas CaO concentration in the reaction mixture was within 2 wt% and 10 wt%. It is shown that calcination temperature strongly influences the final catalyst form, whereby the temperature higher than 700 °C leads to the destruction of the initial zeolitic support and interaction of CaO with the melted glassy silicate phase making less-active or non-active calcium silicate phases. The highest fatty acid methyl esters content (>97 wt.%) was obtained using a catalyst with 44 wt.% of CaO and calcined at 523 °C under the following reaction conditions, reaction temperature of 60 °C, methanol to oil molar ratio of 1/12, catalyst concentration of 8.8 wt.%, and reaction time of 90 min.

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4-3

**Experimental determination of thermodynamic properties  
and modeling of new choline based ionic liquids**

Ivona Đorđević, Nikola Grozdanić, Ivona Radović  
*University of Belgrade, Faculty of Technology and Metallurgy,  
Karnegijeva 4, 11120 Belgrade, Serbia*

Ionic liquids (ILs) are salts consisted of organic cation and organic or inorganic anion, which are in a liquid state at low temperatures (around or below 373.15K). Big advantages of ionic liquids in general are adjustable thermophysical properties with different composition combinations and low vapor pressure. Because of such characteristics ILs have a very wide range of applications within different industries as ecological alternative for many organic solvents etc. For the needs of this work, new ionic liquids based on choline ions as cations were synthesized, with the aim of adsorbing harmful gases from our environment: cholinium triptophanate and cholinium histidinate. Knowing thermophysical properties of ILs and expanding that database is of great importance for further desing of industrial processes. Density, refractive indices and sound velocity of the mentioned ionic liquids in mixture with water were determined experimentaly using Anton Paar DSA 5000M densimeter connected with Anton Paar RXA 156 refractometer, while dynamic and kinematic viscosity were measured on Anton Paar SVM 3000 viscometer. Measurements were done in the temperature range from 303.15K to 323.15K and at atmospheric pressure with a wide range of concentrations in order to overcome the problem of extremely high viscosities of ILs, but also for possible commercial use of them. Experimental viscosity was correlated using appropriate thermodynamic models given as exponential functions with satisfactory average percent deviation for the needs of chemical industry.

4-4

**Xylanase production from *Penicillium chrysogenum*  
and its application in degradation of agricultural waste**

Olivera Vukoichić, Nataša Šekuljica, Zorica Knežević-Jugović  
*University of Belgrade, Faculty of Technology and Metallurgy,  
Karnegijeva 4, 11120 Belgrade, Serbia*

Enzymatic hydrolysis of lignocellulosic biomass has many benefits. It is eco-friendly, has low carbon footprint and includes selective reactions. Xylanase is the group of enzymes that convert xylan into xylooligosaccharides (XOS). Xylan is the part of hemicellulose, which composes plant cell wall, thus making agricultural residues a good substrate for enzymatic hydrolysis catalysed by xylanase. XOS are dietary fibers which function as prebiotics, they stimulate growth of microbiota that inhibits the gastro-intestinal and vaginal tract. XOS have many health benefits and therefore can be incorporated in various foods, feeds and dietary supplements. The goal of this study was to produce xylanase from *Penicillium chrysogenum*, characterise it and test its efficiency on raw and pretreated wheat chaff. *P. chrysogenum* was obtained from Department of Biochemical Engineering and Biotechnology, Faculty of Technology and Metallurgy, University of Belgrade. Wheat chaff was collected from Agricultural cooperative Mrkšićevi Salaši. Commercial enzymes that were used for determination of pretreated substrates quality were cellulase (Sigma-Aldrich, USA) and xylanase (Sigma-Aldrich, USA). In this experiment we tested 4 different pretreatment methods: hydrothermal, acidic and 2 alkaline. Enzyme was produced by fermentation on wheat bran by *P. chrysogenum* for 6 days. It was determined that the optimal temperature for produced xylanase is 37 °C, pH optimum is 6 and after 5 hours in medium that has pH=6 its activity decreases to 93%. Michaelis-Menten constant ( $K_m$ ) of produced enzyme is 42,504 mg ml<sup>-1</sup>, maximum reaction rate ( $v_{max}$ ) is 2,147 μmol min<sup>-1</sup> and the turnover number of an enzyme ( $k_{cat}$ ) is 4,61 x 10<sup>-6</sup> s<sup>-1</sup>. The content of fibers after the pretreatments was examined and it has shown that hydrothermal and alkaline (15 % NH<sub>4</sub>OH) pretreatment preserved majority of the fiber content in substrate, and therefore is the best for further use. Additionally, enzymatic hydrolysis of raw and pretreated wheat chaff with commercial enzymes cellulase and xylanase has shown that the best substrate are raw, hydrothermally and alkali pretreated chaff. Produced enzyme was mixed with commercial cellulase and when the results of enzymatic hydrolysis by this mix were compared to ones obtained by using commercial mix (xylanase + cellulase) we saw similar trend on our graph, which lead us to conclude that the produced xylanase can replace the commercial one.

4-5

### **Carbon material derived from viscose as adsorbent for chlorpyrifos**

Vedran Milanković<sup>1</sup>, Tamara Lazarević – Pašti<sup>2</sup>

<sup>1</sup>*University of Belgrade, Faculty of Physical Chemistry, Studentski Trg 12, 11000 Belgrade, Serbia,* <sup>2</sup>*University of Belgrade, VINČA Institute of Nuclear Sciences - National Institute of the Republic of Serbia, Mike Petrovica Alasa 12-14, 11000 Belgrade, Serbia.*

Organophosphate compounds are often used in agriculture and control the development of insects. Still, they show harmful effects on the human body and pose a danger to the environment and humans. Chlorpyrifos is an organophosphate compound with a wide application as a very strong insecticide, nematicide and acaricide. However, its toxicity is associated with various psychological, endocrine, hematological, respiratory and reproductive problems. The adsorption of chlorpyrifos on the selected carbon material derived from biomass by carbonization of viscous fibers was investigated. The chosen carbon material was characterized using: Raman spectroscopy, BET analysis of the material surface, scanning electron microscopy (SEM) and electron dispersive X-ray spectroscopy (EDX). The concentration of chlorpyrifos was determined using UPLC analysis. We used different concentrations of carbon material at various temperatures and under dynamic and static conditions to examine its efficiency and potential application in chlorpyrifos remediation. The optimal incubation time required to reach adsorption equilibrium was determined by recording UPLC chromatograms after different chlorpyrifos and carbon material contact periods. The determination of the adsorption rate constant was determined by the Guggenheim method. The assessment of the toxicity of the treated sample was monitored by measuring the acetylcholinesterase activity. It was shown that investigated material has a significantly ordered structure and high level of graphitization. Also, specific surface area and total pore volume are relatively large, relatively small pores are dominant, and the viscous fiber retained its primary structure despite carbonization. Comparing the results obtained under static and dynamic conditions, it was concluded that removing chlorpyrifos from water is possible in both experimental setups with nearly the same efficiency. Furthermore, the toxicological analysis showed a decrease in the toxicity of treated aqueous solutions compared to non-treated samples. Thus, it confirms that there was no formation of more toxic products. The investigated material showed the best adsorption efficiency for chlorpyrifos in a concentration of  $1\text{gdm}^{-3}$  at a temperature of  $25\text{ }^{\circ}\text{C}$  under static conditions.

4-6

**Application of DInSAR Technology for Monitoring the Subsidence  
Induced by Salt Mining in Tuzla, Bosnia and Herzegovina**

Bojana Grujić<sup>1</sup>, Žarko Grujić<sup>1</sup>

University of Banja Luka, Faculty of Architecture, Civil Engineering and Geodesy,  
Banja Luka /*Department of Civil Engineering*

Tuzla is well known with salt mining. Previous research found that the massive exploitation activities of salt mining causes ground subsidence up to 12 meters. This result was obtained by analysis of time series topographical data from 1956 to 2003. Abandonment of salt exploitation in centre of Tuzla was lasting from 2001 and finally finished in 2007. The subsidence causes damage to the buildings and infrastructures. Another research using GPS survey revealed that the subsidence was on going during 2004 to 2007. The GPS result shows the subsidence was decreasing. However, the subsidence is still on going in center of Tuzla City especially in the areas near new salt-water lake for swimming.

In this research, we applied Differential Interferometry Synthetic Aperture Radar (DInSAR) method to measure the present subsidence in Tuzla. The main purpose of this research is to enhance the ground subsidence information on spatial distribution and temporal transition. The Small Baseline Subset (SBAS) time series approach is employed. We used Sentinel-1 data from October 2014 to November 2017 to generate the time series of ground subsidence. DInSAR result shows the ground subsidence is still on going in some areas. The maximum subsidence velocity is about 40 mm/year. It means continuous subsidence monitoring is very important. In addition, a comparison of subsidence obtained by DInSAR and GPS is analyzed and discussed in this paper.

5-1

**Effective sorption of toxic brilliant green  
using lignocellulosic waste biomasses and derived biochar samples**

Anja Antanasković<sup>1</sup>, Zorica Lopičić<sup>1</sup>, Tatjana Šoštarić<sup>1</sup>,

Jelena Milojković<sup>1</sup>, Vladimir Adamović<sup>1</sup>, Kristina Vučković<sup>2</sup>, Milan Milivojević<sup>2</sup>

<sup>1</sup>*Institute for Technology of Nuclear and Other Mineral Raw Materials, Belgrade, Serbia,*

<sup>2</sup>*Faculty of Technology and Metallurgy, University of Belgrade, Serbia*

Lignocellulosic waste biomass (LCW) certainly represents a part of the solutions to the low-carbon future. LCW could serve as a base for a variety of sustainable fuels and bio based materials, whose proper implementation could help in economic and environmental growing world demands. Fruit stones, wastes from food processing industries, are contributing toward negative effects on the environment systems through the impacts associated with both waste production and its disposal. This waste type can be converted into value-added products using thermochemical methods, such as pyrolysis, where the biomass is efficiently converted into biofuels, biochars and different value added products. In this paper, two LCW materials, peach (PS) and cherry stones (CS) and their derived biochars (PS-B and CS-B), have been successfully applied for the removal of the hazardous water-soluble cationic dye, brilliant green (BG). Functional groups present in LCWs and related biochars were analysed using Fourier transform infra-red (FTIR) technique. Bio based sorbents were also characterized by determination of pH<sub>sus</sub> and pH<sub>pzc</sub>. The pristine LCWs, PS and CS, were first milled to desired dimensions, washed and dried at 60 °C. Pyrolysed samples, PS-B and PS-C, were obtained by heating in oxygen limited conditions from 25 to 500 °C (10 °C/min heat flow), and kept at 500 °C for 2 h. The contact pH (pH<sub>sus</sub>) as well as pH<sub>pzc</sub> were higher in both cases for the biochar samples, indicating higher –OH content (confirmed also by FTIR analysis) and favourable surface for cationic sorbate types. The experimental sorption results indicated that biochars have almost two times higher sorption capacities than the native materials, under the same operational conditions, while the highest binding was achieved by cherry stone biochar, 135.3 mg/g (experimental data modelled by Sips isotherm). Conclusively, the LCWs derived biochars can be efficiently used as an alternative to conventional sorbents in contaminated water treatment.

5-2

**Synthesis of Samarium and Zirconium-doped TiO<sub>2</sub> nanofibers  
with improved photocatalytic activity**

Sanita Ahmetović<sup>1</sup>, Zorka Ž. Vasiljević<sup>1</sup>, Nikola Cvjetičanin<sup>2</sup>,  
Jelena Vujančević<sup>3</sup>, Nenad B. Tadić<sup>4</sup>, Vladimir B. Pavlović<sup>5</sup>, Maria Vesna Nikolić<sup>1</sup>

<sup>1</sup>*University of Belgrade – Institute for Multidisciplinary Research, Belgrade, Serbia,* <sup>2</sup>*University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia,* <sup>3</sup>*ITS SASA, Belgrade, Serbia,* <sup>4</sup>*University of Belgrade, Faculty of Agriculture, Belgrade, Serbia*

Samarium and zirconium-doped TiO<sub>2</sub> nanofibers (3 and 5 wt.%) were synthesised by a simple modified electrospinning method. The effects of calcination temperature on the size of the as-spun doped titania fibers was investigated. As-spun nanofibers were studied and characterized through thermal gravimetric analysis (TG-DTA), Fourier Transform Infrared Spectroscopy (FTIR) and Scanning electron microscopy (SEM), while the structure and morphology of calcined fibers was studied by X-Ray Diffraction (XRD), Field Emission Electron Microscopy (FESEM) and spectroscopic techniques (FT-IR and DRS UV-vis). The influence of dopant type and amount on the photocatalytic degradation of Methylene blue (MB) was investigated.

5-3

**Investigation of biological activity of freeze-dried goat whey  
with the addition of dry spices**

Mihailo Mladenović, Marija Milić, Suzana Dimitrijević-Branković  
*University of Belgrade, Faculty of Technology and Metallurgy,  
Departement of Biochemical Engineering and Biotechnology*

Goat whey is a by-product in the production of goat cheese and casein from goat's milk. Its positive effect on human health is increasingly being investigated, which is why it is recognized as an exceptional raw material for the production of biotechnological products in the food industry.

The aim of this work was to determine the effect of the supplementation of dried herbs on the antioxidant, antimicrobial and prebiotic activity of lyophilized goat whey.

Four samples of goat whey with the addition of ashwagandha (*Withania somnifera*), ramsons (*Allium ursinum*) and a mixture of turmeric (*Curcuma longa*) and black pepper (*Piper nigrum*) were extracted by microwave-assisted extraction using water as solvent. The content of total polyphenols was determined in the obtained supernatants and the antioxidant properties were measured by DPPH and FRAP method, as well as antimicrobial and prebiotic properties by the method of dilution on agar-agar medium. Bacteria *Escherichia coli* and *Staphylococcus aureus*, together with pathogenic yeast *Candida albicans* were used for antimicrobial testing, while bacteria *Lactobacillus rhamnosus* and probiotic yeast *Saccharomyces cerevisiae* var. *boulardii* were used for prebiotic activity.

The results of this study showed that herbal supplements improved the antioxidant properties of goat whey. The highest antioxidant activity was shown by the sample of whey supplemented with ramsons, which was twice as high as whey without additives, while the content of total polyphenols was higher by 54%. Determining antimicrobial activity, the samples showed complete inhibition of *E. coli* and *S. aureus*, while the degree of growth inhibition of *C. albicans* was 20-41%, depending on the type of sample. Measuring prebiotic activity, the results showed that the samples did not affect the growth stimulations of the examined microorganisms. However, the sample of whey with the addition of ramsons was distinguished, which showed a certain degree of growth inhibition of *L. rhamnosus* GG (40%), which is interesting because the same sample showed the highest degree of inhibition of *C. albicans* (41%). The obtained results may be of great importance for the further development of the food industry, having in mind the significant improvement of the quality of goat whey as a raw material.

5-4

### **Europium-doped manganese tungstate for dual electrocatalytic activity**

Andrej Kukuruzar<sup>1</sup>, Slađana Savić<sup>1</sup>, Filip Vlahović<sup>2</sup>, Dalibor Stanković<sup>1,3</sup>

<sup>1</sup>*University of Belgrade, Faculty of Chemistry, Studentski trg 12-16, 11000, Beograd, Serbia,*

<sup>2</sup>*Innovation Center of the Faculty of Chemistry, University of Belgrade, Serbia,* <sup>3</sup>*'VINČA'  
Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of  
Belgrade, Belgrade, Serbia*

Ethidium bromide (EthBr) is a fluorescent dye commonly used in molecular biology for visualization of DNA in electrophoresis gels. As EthBr intercalates nucleic acids, it is a potential human mutagen. Therefore, an efficient method for its removal would be beneficial to human and environmental safety.

Europium(III)-doped manganese tungstate was synthesized and characterized. The Eu-doped  $\text{MnWO}_4$  and modified carbon paste electrodes (CPE) containing different amounts of this material were characterized. These electrodes were used for electrochemical determination and degradation of EthBr.

Firstly, EthBr was characterized electrochemically by cyclic voltammetry using a glassy carbon electrode and the different CPEs, at different conditions. Then, the optimal method for voltammetric EthBr determination using the modified CPE was investigated. It was found that SWV gives the best results.

Lastly, the material was applied to graphite rods as electrodes for electrochemical oxidative removal of EthBr from aqueous solution and the optimal parameters for the process were established. The resulting degradation products were determined. The devised method gave satisfying results for dye removal, with complete decolorization after 50 minutes of treatment.



5-5

### **Thermally activated pyrophyllite as ceramic membrane**

Katarina Tošić<sup>1</sup>, Bojana Paskaš Mamula<sup>1</sup>, Nikola Novaković<sup>1</sup>, Mirjana Medić Ilić<sup>1</sup>,  
Igor Milanović<sup>1</sup>, Silvana Dimitrijević<sup>2</sup>, Jasmina Grbović Novaković<sup>1</sup>

<sup>1</sup>*Centre of Excellence for Hydrogen and Renewable Energy, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, POB 522 Belgrade, Serbia,* <sup>2</sup>*The Mining and Metallurgy Institute Bor, Zeleni bulevar 35, 19210 Bor, Serbia*

Due to pyrophyllite good physico-chemical characteristics, such as low electrical and thermal conductivity, good mechanical strength, low coefficient of expansion and excellent stability during heat treatment, it is widely used in many industries, such as industry paper, plastic, ceramics, rubber, plants, bricks and cosmetics, but also for waste treatment water. In this paper, the thermal modification of pyrophyllite is performed at a temperature of 1050 °C in a time interval of 2-6 h, under a pressure of 50 MPa, in order to obtain ceramic membranes for purification of pollutants in aqueous solutions. Prior to thermal treatment natural pyrophyllite clay is ultrasonically purified to remove other impurities. The changes that occurred after the thermal treatment were monitored: X-ray structural analysis (XRD), infrared spectroscopy with Fourier transform (FTIR), scanning electron microscopy (SEM), Raman spectroscopy, as well as thermal methods of analysis, which monitored the thermal stability of the obtained material.

5-6

**Effects of sulphur hexafluoride cold plasma hydrophobization  
on the polyoxymethylene surface**

Michał Chodkowski<sup>1</sup>, Zoltan Károly<sup>2</sup>, Szilvia Klébert<sup>2</sup>, Konrad Terpiłowski<sup>1</sup>

<sup>1</sup>*Department of Interfacial Phenomena, Institute of Chemical Sciences,  
Faculty of Chemistry, Maria Curie-Skłodowska University in Lublin (UMCS),  
pl. Marii Curie-Skłodowskiej 3, 20-031 Lublin, Poland,* <sup>2</sup>*Institute of Materials and  
Environmental Chemistry, Research Centre for Natural Sciences, Magyar tudósok körútja 2,  
H-1117 Budapest, Hungary*

Polyoxymethylene, known also as POM or polyacetal, is an important engineering polymer. It is composed of successive C-O bonds in the main chain which form oxymethylene units (–CH<sub>2</sub>O–). POM is an engineering thermoplastic used wherever great stiffness and small friction as well as excellent dimensional stability play a key role. One of the methods for improvement of the surface properties is the material modification with plasma. The effect depends on the carrier gas used for the plasma generation because the ionized substrate has the ability to react with the surface. In the case of the fluorinated gases there can be an increase in the surface hydrophobicity due to the incorporation of halogen derivatives.

In this paper the polymer surface was modified with the SF<sub>6</sub> cold plasma using different values of parameters such as process time, generator power or gas flow. Then the obtained surfaces were characterised using the contact angle measurements (wettability and surface free energy calculations), X-ray photoelectron spectroscopy (changes in the surface chemistry) as well as optical profilometry (surface topography and roughness).

It was found that highly hydrophobic, self cleaning surfaces were obtained. They are featured by the contact angle up to 140 degrees as well as low tilting angle smaller than 10 degrees. Moreover, the surface wettability was related to its roughness and topography.

6-1

**Effect of processing parameters on NaGdYF<sub>4</sub>:Yb,Er UCNPs  
structural, morphological and optical properties**

Ivana Dinic<sup>1</sup>, Marina Vukovic<sup>2</sup>, Marko Nikolic<sup>3</sup> and Lidija Mancic<sup>1</sup>

<sup>1</sup>*Institute of Technical Sciences of SASA, Belgrade, Serbia*

<sup>2</sup>*Innovative Centre, Faculty of Chemistry Belgrade, University of Belgrade, Serbia*

<sup>3</sup>*Photonic Center, Institute of Physics Belgrade, University of Belgrade, Serbia*

Synthesis of monosized and spherical Up-Converting NanoParticles (UCNPs) with biocompatible surface are of a great interest because of their potential application in biomedicine as biomarkers or drug delivery systems. Among different synthesis routes reported in the literature, a hydro/solvo thermal method is considered to be most potential one for scaling-up due to the fact that it is simple and economically cost-effective. In this work the synthesis of NaY<sub>0.65</sub>Gd<sub>0.15</sub>F<sub>4</sub>:Yb,Er UCNPs were performed through chitosan assisted solvothermal synthesis at 200°C. Variation of precursors concentration, type of solvent and synthesis time were performed in order to explore their influence on the structural, morphological and optical properties of the UCNPs. The XRD analysis showed that with a smaller surplus of fluoride ions the formation of Y<sub>0.65</sub>Gd<sub>0.15</sub>F<sub>4</sub>:Yb,Er orthorhombic phase occurs, while the increase of fluoride content or reaction time leads to NaY<sub>0.65</sub>Gd<sub>0.15</sub>F<sub>4</sub>:Yb,Er cubic phase formation. Along with it, the changes of UCNPs morphology from spindle to spherical shape is detected. All samples emit intense green emission due to the (<sup>2</sup>H<sub>11/2</sub>, <sup>4</sup>S<sub>3/2</sub>) → <sup>4</sup>I<sub>15/2</sub> electronic transitions, after being excited with infrared light (λ=978 nm).

6-2

**Electrochemical synthesis of silver nanoparticles in poly(vinyl alcohol)-based hydrogels and evaluation of their sizes by comparing experimental and simulated UV-visible spectra**

Marko Opsenica, Katarina Nešović, Vesna Mišković-Stanković  
*University of Belgrade, Faculty of Technology and Metallurgy,  
Karnegijeva 4, Belgrade, Serbia*

Due to their biocompatibility and non-toxicity, hydrogels have found many different applications in medicine. Extremely important properties of hydrogels such as the ability to absorb significant amounts of liquid, as well as the ability for controlled release of drugs incorporated inside the hydrogel matrices, have prompted their usage as biocompatible wound dressing materials. Of particular importance for medical applications is the ability of hydrogels to incorporate antibacterial agents, such as silver nanoparticles (AgNPs). In this work, AgNPs were electrochemically incorporated inside the poly(vinyl alcohol) (PVA) based hydrogels, also containing chitosan (CHI) and graphene (Gr), previously swollen in  $\text{AgNO}_3 + \text{KNO}_3$  solution. Electrochemical reduction is an efficient and environment-friendly *in situ* method for obtaining AgNPs of small dimensions, directly inside the hydrogel matrix. The AgNPs-loaded hydrogels were synthesized at constant voltages of 50 V, 70 V, 90 V, and 110 V, in order to discern the optimal synthesis conditions. The efficient silver nanoparticles incorporation was confirmed by characteristic UV-visible absorption maxima in the wavelength range of 398-406 nm. Simultaneously, theoretical simulations of the AgNPs absorption spectra were performed using the MiePlot software. By comparison of the experimentally obtained and simulated spectra, diameters of the obtained silver nanoparticles were estimated to be between 39.0 and 51.5 nm, depending on the applied voltage, synthesis duration and hydrogel composition. Based on the obtained results, it was concluded that the optimal voltages for nanoparticle synthesis in silver/poly(vinyl alcohol)/chitosan hydrogels were 50 V and 90 V, as these samples exhibited the highest amounts of incorporated silver nanoparticles with the smallest diameters. This was also confirmed for the silver/poly(vinyl alcohol)/chitosan/graphene hydrogel, which was synthesized at 90 V.

6-3

**Radiation-chemical synthesis of antibacterial  
Ag-poly(vinyl alcohol)/poly(N-vinyl-2-pyrrolidone) nanocomposite hydrogels**

Nikolina Nikolić, Jelena Spasojević, Aleksandra Radosavljević, Zorica Kačarević-Popović  
*Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University  
of Belgrade, Belgrade, Serbia*

Hydrogel/metal nanocomposites, as a special group of biomaterials, have become the subject of extensive research in material science. Among various techniques, the radiation-chemical method is very suitable for crosslinking of polymer matrix as well as for *in situ* formation of metal nanoparticles in the hydrogel by radiolytic products of water. This technique does not require any harmful substances and does not need any further purification, which makes it a "green" method. This work describes the radiation-chemical synthesis of silver nanoparticles (Ag NPs) within hydrogels based on poly(vinyl alcohol) (PVA) and poly(N-vinyl-2-pyrrolidone) (PVP). A series of PVA/PVP hydrogels with different compositions were previously obtained by gamma-irradiation-induced crosslinking, and their porous sponge-like structure was observed by SEM analysis. The liquid filled cavities, inside such type of structure, serve as nanoreactors for *in situ* synthesis of NPs. The formation of highly stable and uniformly distributed Ag NPs has been confirmed by UV-VIS spectroscopy. A strong characteristic surface plasmon resonance was in the range of 390-420 nm, indicating the average size of Ag NPs from 9 nm up to 14 nm. The XRD measurement revealed the face centered cubic (*fcc*) crystal structure of Ag NPs, with the average crystalline domain size around 10 nm. The PVA/PVP polymer matrix binding environment of the AgNPs was examined by X-ray photoelectron spectroscopy. FTIR spectra indicate that incorporation of Ag NPs into PVA/PVP hydrogel decrease intensity of characteristic vibration, in comparison with PVA/PVP hydrogel, due to formation of a coordinate bond between the polymer chains and NPs. The swelling capacity and swelling kinetic parameters are some of the basic properties of hydrogels from the potential biomedical applications point of view. The swelling curves analysis show that the presence of Ag NPs in hydrogel matrix changes the diffusion type from non-Fickian diffusion for PVA/PVP hydrogels to Fickian diffusion for Ag-PVA/PVP nanocomposite hydrogels. Finally, the appearance of inhibition zone around tested Ag-PVA/PVP nanocomposite hydrogels clearly indicates the good antibacterial effect against investigated bacteria, *Escherichia coli* and *Staphylococcus aureus*, and suggests that can be a good candidate for biomedical applications (wound dressing or drug delivery systems).

6-4

**Synthesis of nano-sized  $\text{NiMn}_2\text{O}_4$  by glycine nitrate  
and electrospinning processes and its pseudocapacitive behavior**

Milena Dojčinović<sup>1</sup>, Zorka Ž. Vasiljević<sup>1</sup>, Nenad Tadić<sup>2</sup>, Jugoslav Krstić<sup>3</sup>,  
Smilja Marković<sup>4</sup>, Matiaž Spreitzer<sup>5</sup>, Janez Kovač<sup>5</sup>, Maria Vesna Nikolić<sup>1</sup>

<sup>1</sup>*University of Belgrade – Institute for Multidisciplinary Research, Belgrade, Serbia,*

<sup>2</sup>*University of Belgrade, Faculty of Physics, Belgrade, Serbia,* <sup>3</sup>*University of Belgrade, IChTM, Belgrade, Serbia,* <sup>4</sup>*ITS of SASA, Belgrade, Serbia,* <sup>5</sup>*Institute Jožef Štefan, Ljubljana, Slovenia*

$\text{NiMn}_2\text{O}_4$  was synthesized with two synthetic routes: sol-gel combustion method with glycine as fuel and electrospinning method with polyvinylpyrrolidone (PVP) as polymer carrier for metal precursors. Amorphous powders from sol-gel synthesis were calcined at 800 °C. As-spun fibers were characterized with TG/DTA to investigate adequate calcination temperature that was then set to 400 °C. Structural analysis of synthesized powders was done via X-ray diffraction (XRD) and results show spinel structure with no impurity. The texture and morphology was investigated via  $\text{N}_2$  physisorption and transmission electron microscopy (TEM). Oxidation states of elements were investigated by X-ray photoelectron spectroscopy (XPS). The electrochemical performance of the synthesized materials as supercapacitors was tested via cyclic voltammetry (CV), electric impedance spectroscopy (EIS), and chronopotentiometry (CP). The results show good capacitance values.

6-5

**Characterization of a new Yb<sup>3+</sup>/Er<sup>3+</sup> doped SrGd<sub>2</sub>O<sub>4</sub> up-conversion nanomaterial obtained via glycine-assisted combustion synthesis**

Tijana Stamenković<sup>1</sup>, Nadežda Radmilović<sup>1</sup>, Marija Prekajski-Đorđević<sup>2</sup>,  
Ivana Dinić<sup>3</sup>, Lidija Mančić<sup>3</sup>, Vesna Lojpur<sup>1</sup>

<sup>1</sup>*Department of Atomic Physics, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, P.O. Box 522, 11001 Belgrade, University of Belgrade, Serbia*

<sup>2</sup>*Department of Materials, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, P.O. Box 522, 11001 Belgrade, University of Belgrade, Serbia*

<sup>3</sup>*Institute of Technical Science of SASA, Knez-Mihailova 35/4, Belgrade, Serbia*

In this work we present new up-conversion materials, consisted of SrGd<sub>2</sub>O<sub>4</sub> matrix co-doped with different Yb<sup>3+</sup> (1, 2.5 and 5 at%) and constant Er<sup>3+</sup> (0.5 at%) concentrations, prepared by glycine-assisted combustion method. X-ray powder diffraction (XRPD) showed that as-synthesized nanoparticles have orthorhombic structure (Pnma), assigned to the JCPDS Card No:01-072-6387. Rietveld refinement indicated a decrease in the size of the unit cell, lattice parameters, and cell volume, due to successful doping of Yb<sup>3+</sup> and Er<sup>3+</sup> ions into the matrix. Transmission electron microscopy (TEM) revealed that obtained nanostructure is composed of agglomerated nanoparticles, while energy dispersive spectroscopy (EDS) confirmed uniform distribution of all constituting elements in them. Up-conversion (UC) luminescence spectra measured in function of laser pumping power indicated that two-photon UC process is established in nanoparticles as a result of the trivalent erbium f-f electronic transitions: there are two green emission bands at 523 and 551 nm (<sup>2</sup>H<sub>11/2</sub>, <sup>4</sup>S<sub>3/2</sub> → <sup>4</sup>I<sub>15/2</sub>) and a red emission band at 661 nm (<sup>4</sup>F<sub>9/2</sub> → <sup>4</sup>I<sub>15/2</sub>). The rise of Yb<sup>3+</sup> concentration from 1 to 5 at% provokes a considerable change of the green to red ratio which indicates the possibility to optimize the color output.

6-6

**Improving the compatibility of zirconium oxide nanoparticles and styrene-free polyester resin by coupling with vinyl functionalized silane**

Jelena D. Gržetić<sup>1</sup>, Slavko Mijatov<sup>1</sup>, Marica Bogosavljević<sup>1</sup>,  
Tihomir Kovačević<sup>1</sup>, Saša Brzić<sup>1</sup>

*Military Technical Institute, Ratka Resanovića 1, Belgrade, Serbia*

In this study, the zirconium oxide nanoparticles ( $n\text{-ZrO}_2$ ) are coated using silane coupling agent (vinyltriethoxysilane, VTES) by hydrolysis and condensation reactions in order to improve the compatibility with styrene-free polyester resin (UPe) and achieve higher mechanical performances. Nanocomposites based on styrene-free UPe and unmodified or VTES-coated  $\text{ZrO}_2$  nanoparticles are prepared using solution blending method. FT-IR spectra of uncoated and VTES-coated  $\text{ZrO}_2$  nanoparticles are investigated to confirm the coating efficiency of VTES on  $\text{ZrO}_2$  surface. Uniaxial tensile tests confirm that loading of 1.5 wt.% VTES-coated  $\text{ZrO}_2$  nanoparticles causes increase in tensile strength for 176%. The similar improving of tensile strength is achieved with 5 wt.% unmodified  $\text{ZrO}_2$  nanoparticles. Reinforcing efficiency is determined using dynamic-mechanical analysis, and the highest increase (12.4%) is observed in composites with 5 wt.% of VTES-coated  $\text{ZrO}_2$  nanoparticles.



7-1

### **Graphene quantum dots with amino groups as a potential photoluminescent probe for Fe(III) ions**

Sladana Dorončić<sup>1</sup>, Olivera Marković<sup>2</sup>, Duška Kleut<sup>1</sup> and Svetlana Jovanović<sup>1</sup>

<sup>1</sup>*Vinča”-Institute of Nuclear sciences - National Institute of the Republic of Serbia,  
University of Belgrade P.O. Box 522, 11001 Belgrade, Serbia,*

<sup>2</sup>*University of Belgrade-Institute of Chemistry, Technology and Metallurgy, Department of  
Chemistry, Njegosëva 12, 11000 Belgrade, Republic of Serbia*

In the era of pollution and hazardous materials, new methods for the detection of pollutants in the environment are urgently needed. Due to their specific features such as photoluminescence (PL) in the visible part of the spectrum, dispersibility in water, and organic solvents, nontoxicity, and biocompatibility, graphene quantum dots (GQDs) attract attention in optical sensing of various ions and molecules. In this study, pristine graphene quantum dots (p-GQDs) were produced in a simple single-step electrochemical top-down approach using graphite electrodes as a starting material, and dispersion of sodium-hydroxide in 96% ethanol as a medium for electrochemical reaction. These p-GQDs were gamma-irradiated in a dose of 25 kGy in presence of ethylenediamine in Ar medium to introduce amino groups in their crystal lattice. Results obtained from AFM microscopy indicate the height-uniformity of irradiated GQDs. The presence of amino groups in GQDs was confirmed by FTIR, XPS, and UV-Vis spectroscopies. According to results obtained from PL spectroscopy, a significant narrowing of emission band in irradiated GQDs was observed. In further research, these GQDs were investigated as a potential PL sensor for iron which is one of the most abundant heavy metal in the environment. In the preliminary investigation, a water dispersion of irradiated GQDs was mixed with Fe(III) solution in concentrations of 50 and 100  $\mu\text{M}$ . Using a PL spectroscopy the PL intensity of irradiated GQDs in presence of Fe (III) was measured. From the obtained results, it can be seen that Fe(III) ions lead to quenching of GQDs PL intensity. Then, PL intensities were measured in presence of Fe(III) ions in concentration range 0-100  $\mu\text{M}$ . With an increase of Fe(III) concentration, the PL intensity of GQDs decreased. It can be concluded that gamma-irradiated amino-doped GQDs have significant potential in the so-called „turn of“ detection of Fe(III) ions in the aqueous medium.

**Acknowledgments:** This work was financially supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. 451-03-9/2021-14/200017, 451-03-9/2021-14/200026).

7-2

### **Nanocomposite graphene oxide/silver nanowires: structural and morphological analysis**

Aleksandra Mišović<sup>1</sup>, Danica Bajuk Bogdanović<sup>2</sup>, Milica Budimir<sup>1</sup> and Svetlana Jovanović<sup>1</sup>  
<sup>1</sup>*“Vinča” Institute of Nuclear Sciences - National Institute of the Republic of Serbia,*  
*University of Belgrade, P.O. Box 522, 11000 Belgrade, Serbia,* <sup>2</sup>*Faculty of Physical*  
*Chemistry, University of Belgrade, P.O. Box 47, 11158 Belgrade, Serbia*

A graphene oxide (GO) and silver nanowire (AgNW) nanocomposites show broad range of potential applications from electronics to biomedicine, with arising interest for electromagnetic interference (EMI) shielding. In a form of the free-standing film, composite can be used as a filter membrane or a coating. It is known that the reduction of GO can improve the properties of the material. For the preparation of the free-standing films, GO was synthesized by Hummer's method through oxidation of graphite, while AgNW have been synthesized by a polyol process. A dispersion of GO with 37.5% AgNW was made. The free-standing films were obtained by depositing the dispersion on a filtration system. A dispersion of GO without AgNW was used for the preparation of the reference free-standing film in the same way. The films were chemically reduced with ascorbic acid and elevated temperature. For the treated and untreated films the following characterizations were performed: Raman spectroscopy for structure analysis, atomic force microscopy (AFM) for morphology and roughness analysis, and four-point probes measurement for electrical conductivity analysis. Raman spectra of composite present D and G peaks centered at  $\sim 1350\text{ cm}^{-1}$  and  $\sim 1600\text{ cm}^{-1}$ , respectively, and a second-order band centered at  $\sim 2900\text{ cm}^{-1}$ . The relative intensity ratio of the D and G bands decreased after the reduction from 1.02 to 0.70, which can be attributed to the partial restoration of  $\text{sp}^2$  structures during the deoxygenation process. Based on AFM analysis, the surface roughness of the composite was determined as ISO grade numbers N5 (mean roughness (Ra) 460 nm). The results of the four-point probes measurement before and after reduction showed that the reduction improved the electrical conductivity of the composite more than 5 times (the electrical resistance decreased from  $165\text{ }\Omega/\square$  to  $32\text{ }\Omega/\square$ ). These results proved the successful removing of O-functional groups from GO structure. Acknowledgments: This work was financially supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. 451-03-9/2021-14/200017).

7-3

**Investigation of the interaction of graphene oxide  
and 12-tungstophosphoric acid in aqueous suspensions**

Milica Pejčić<sup>1</sup>, Željko Mravik<sup>1</sup>, Danica Bajuk-Bogdanović<sup>2</sup>, Snežana Uskoković-Marković<sup>3</sup>,  
Bojana Nedić Vasiljević<sup>2</sup>, Sonja Jovanović<sup>1</sup>, Zoran Jovanović<sup>1</sup>

<sup>1</sup>*Laboratory of Physics, Vinča Institute of Nuclear Sciences – National Institute of the  
Republic of Serbia, University of Belgrade, Belgrade, Serbia,*

<sup>2</sup>*Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia,*

<sup>3</sup>*Faculty of Pharmacy, University of Belgrade, Belgrade, Serbia*

Graphene oxide (GO) and 12-tungstophosphoric acid (WPA) nanocomposites (5 to 50 wt.% of WPA, nominally) were prepared and the nature of the interaction between components in suspension is explored from the aspect of surface chemistry. Two methods of functional group modification were selected: chemical titration (NaOH, Na<sub>2</sub>CO<sub>3</sub>, NaHCO<sub>3</sub>) and thermal treatment (T=450 °C, in Ar), while Fourier-transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), temperature programmed desorption (TPD), zeta-potential and adsorption of methylene-blue measurements were used for monitoring the changes of surface chemistry. FTIR results have shown the removal of C=O (1720 cm<sup>-1</sup>) and C-O (1060 cm<sup>-1</sup>) functional groups both in the case of titrated and thermally treated samples. Also, FTIR has shown that thermal treatment did not cause structural changes of WPA in the composite, while this was observed in the case of titration, probably as a consequence of the change of the pH. XPS showed that titration and thermal treatment of GO and GO/WPA (15 wt.%) removes C-O groups approximately to the same extent, while the ratio of COOH and C=O groups in both cases is unchanged compared to initial samples. TPD results showed that the amount of groups removed by titration is smaller compared to thermal treatment, which can be attributed to selectivity of titrant. Zeta-potential measurements have shown that stability of suspensions is improved as the amount of WPA increases. Also, more negative values of zeta-potential were observed as pH increased, which can be attributed to proton consumption during titration. Color adsorption has shown that functional groups of GO have a positive effect, since their removal reduces the adsorption capacity of the material. In the case of nanocomposite, the presence of WPA is beneficial since adsorption capacity is improved compared to the starting GO. Also, it can be concluded that titration improves the adsorption capacity, while thermal treatment completely blocks the adsorption properties of the composite. This is an interesting observation and will be explored in more detail in the future.

7-4

**Surface, structural and electric properties  
of ion beam irradiated graphene oxide papers**

Željko Mravik<sup>1</sup>, Marko Gloginjić<sup>1</sup>, Danica Bajuk-Bogdanović<sup>2</sup>, Maria Vesna Nikolić<sup>3</sup>,  
Andrzej Olejniczak<sup>4,5</sup>, Nemanja Gavrilov<sup>2</sup>, Zoran Jovanović<sup>1</sup>

<sup>1</sup>*Center of Excellence for Hydrogen and Renewable Energy (CONVINCE), Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia;*

<sup>2</sup>*Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia;* <sup>3</sup>*Institute for Multidisciplinary Research, University of Belgrade, Serbia;* <sup>4</sup>*Flerov Laboratory of Nuclear Reactions, Joint Institute for Nuclear Research, Dubna, Moscow region, Russia;* <sup>5</sup>*Faculty of Chemistry, Nicolaus Copernicus University, Toruń, Poland*

Graphene oxide (GO) has emerged as a promising material for electrochemical charge storage due to its high capacitance originating from all-surface morphology and different oxygen groups that participate in redox reactions. Ion beam irradiation can be identified as a technique where a controllable change of surface chemistry and structure of GO is possible through varying the energy and the fluence of an ion beam. In the present study, the influence of keV-energy ion-beam irradiation on the surface chemistry, structural and electrical properties of GO paper were investigated. The results of X-ray photoelectron spectroscopy and Fourier-transform infrared spectroscopy showed an increasing reduction of GO and the preferential removal of the alkoxy and epoxy groups with increasing fluence. Raman analysis showed that there is clear correlation between oxygen content and structural parameters of the irradiated GO. Electric properties of ion beam irradiated GO papers were investigated using the solid-state electrochemical impedance spectroscopy (EIS) and compared to the effects of thermal treatment. With irradiation, lower resistivity of GO papers was observed with fluencies up to  $1 \times 10^{16}$  ions/cm<sup>2</sup> proving that desorption of basal plane oxygen groups is beneficial for improvement of electric characteristics of material. At higher fluence, a higher defect concentration resulted in an increase of resistivity of the irradiated samples. Additionally, EIS results outlined a different behavior of ion beam irradiated and thermally treated samples (capacitor vs. resistor, respectively), originating from the different extent of modification (ion beam irradiation – modification of few hundred nm and thermal treatment – bulk modification).

7-5

**Hydrothermal synthesis and characterization of composite of graphene oxide and cobalt ferrite doped with zinc and gallium**

Marija Grujičić<sup>1,2</sup>, Ivana Stojković Simatović<sup>1</sup>, Danica Bajuk Bogdanović<sup>1</sup>,  
Zoran Jovanović<sup>2</sup>, Željko Mravik<sup>2</sup>, Sonja Jovanović<sup>2</sup>

<sup>1</sup>*Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia,*

<sup>2</sup>*“VINČA” Institute of Nuclear Sciences – National Institute of the Republic of Serbia,  
University of Belgrade, Belgrade, Serbia*

In this paper, the physicochemical properties of nanocomposites of graphene oxide (GO) and cobalt ferrite nanoparticles CFO NPs (pristine and doped with zinc and gallium, CFO\_Zn, CFO\_Ga) were investigated. CFO, CFO\_Zn and CFO\_Ga NPs were synthesized using the solvothermal method with oleic acid (OA) as a surfactant. X-ray diffraction (XRD) confirmed the presence of pure ferrite phase while transmission electron microscopy (TEM) revealed spherical and non-agglomerated NPs with average size of  $5 \pm 1$  nm. Fourier transform infrared spectroscopy (FTIR) has confirmed bridging bidentate interaction between the oleic acid and the metal atoms on the surface of the NPs, while Raman spectroscopy results confirmed the incorporation of zinc and gallium in the spinel structure. Prior to preparation of nanocomposite with GO, an OA coating has been exchanged with dihydrocaffeic acid (DHCA). DHCA binds to surface of NPs through both covalent bridging bidentate interaction and catechol groups, as determined by FTIR. Nanocomposite has been obtained by adding CFO(\_Zn/Ga) NPs to a GO suspension with nominal fractions of 5 to 15 wt.%, followed by homogenization and hydrothermal treatment ( $T=120$  °C,  $t=3$  h). TEM results revealed that the shape and size of NPs remain unchanged in nanocomposite, while FTIR results have shown that hydrogen bond is established between the functional groups of GO and DHCA. Electrochemical properties of individual components and nanocomposite were examined by cyclic voltammetry. The best electrochemical properties, in terms of the highest specific capacity, were shown by the composite which contains 15 wt.% CFO NPs.

7-6

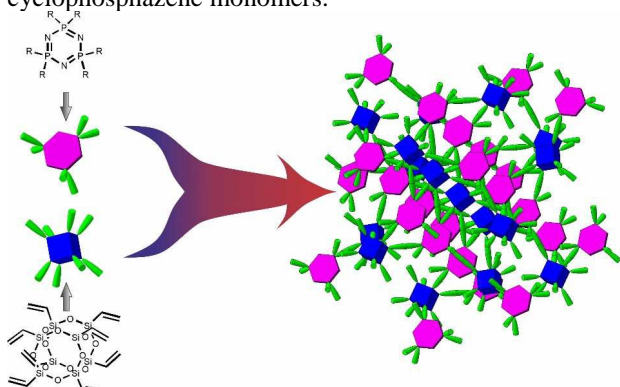
### Hybrid functional porous polymers, based on phosphazene and cage-like siloxane building blocks

Mikhail Soldatov<sup>1</sup>, Anna Chernysheva<sup>1</sup>, Hongzhi Liu<sup>2</sup>, Sergei Kostjuk<sup>3</sup>

<sup>1</sup>*D. Mendeleev University of Chemical Technology of Russia, Moscow, Russian Federation,*

<sup>2</sup>*Shandong University, Jinan, People Republic of China, <sup>3</sup>Belarussian State University, Minsk, Republic of Belarus*

Porous polymers are of a great interest due to their high surface area and have found application in various fields such as catalysis, adsorbents, sensors etc. During the past decades the interest in preparation of porous materials with the use of cage-like siloxane building blocks is growing. Such interest is explained by the unique properties of the building blocks, especially their hybrid inorganic-organic nature providing high thermal and chemical stability on the one hand and possibility for further functionalization on the other hand. Moreover the rigid structure of such monomers provides the high porosity during the cross-linking process. Phosphazene building blocks also possess unique properties due to hybrid nature and due to high basic properties of the nitrogen atoms in phosphazene backbone. Here we prepared various porous polymers by cross-linking the cage-like siloxane and cyclophosphazene monomers.



The obtained porous polymers are promising as effective adsorbents and catalysts.

7-7

### **Recent Progress of Carbon Dots in Nanomedicine and Photocatalysis**

Yiqun Zhou and Roger M. Leblanc  
*University of Miami, USA*

Carbon dots (CDs) are a group of carbon-based spherical nanoparticles (NPs) with diameters less than 10 nm. They are widely present in the nature and can be also synthesized using various carbon-based substances as precursors by either top-down or bottom-up approaches. They are well characterized for tunable surface functionality, excellent photoluminescence (PL), high photostability and water dispersity, good biocompatibility, and nontoxicity. Also, they display different sizes and surface chemistry depending on the preparation methods and precursors applied. Applications of CDs in drug delivery, bioimaging, sensing, optics, photocatalysis, and other nanotechnology fields are rapidly rising due to their aforementioned unique properties.

In this presentation, I will focus on the development of CDs in our group in nanomedicine and photocatalysis. Specifically, I will present Y-CDs able to cross the blood-brain barrier (BBB) via passive diffusion targeting the generation of amyloid precursor protein (APP) and beta-amyloid ( $A\beta$ ). In addition, carbon nitride dots (CNDs) have shown inhibitory effect on the aggregation of microtubule-associated tau protein, whose structure-function relationship is under investigation. Both projects are significant for the future treatment of Alzheimer's disease (AD). Furthermore, I would like to share with the public that CDs proved to be promising Lego-like building blocks for the assembly of versatile drug nanocarriers to simultaneously fulfill multitasks. Moreover, G-CDs have exhibited excellent photocatalytic reactivity comparable to graphitic carbon nitride, which allows G-CDs to be considered as another metal-free future photocatalyst.

8-1

**Structural, spectroscopic and quantum-chemical investigation  
of testosterone propionate**

Nikola Ristivojević, Dušan Dimić

*University of Belgrade-Faculty of Physical Chemistry,  
Studentski trg 12-16, 11000 Belgrade, Serbia*

Anabolic steroids represent a group of molecules commonly misused in sport because of their effects on the muscular system and weight. Testosterone Propionate (TP) is an anabolic steroid and ester of testosterone. In this contribution, the use of Density Functional Theory (DFT) methods for the possible determination of counterfeit substances such as TP was investigated. The structure was optimized at the B3LYP/6-311++G(d,p) level of theory based on crystallographic data. Small values of Mean Absolute Error (MAE) for bond lengths (0.04 Å) and angles (3°) proved the applicability of the given level of theory, which was later used for the prediction of Raman, IR, NMR, and UV spectra. The most prominent bands in the IR theoretical spectra, positioned at 1730 and 1665 cm<sup>-1</sup>, belong to the stretching vibration of carbonyl groups. Wavenumbers of these vibrations are well-correlated with the bands in the experimental spectra (1710 and 1670 cm<sup>-1</sup>). The optimization of structure in various solvents and prediction of wavenumbers for carbonyl group vibrations showed a 2-20 cm<sup>-1</sup> difference when compared to experimental values depending on the polarity of solvents. The bands representing C-H vibrations are within ≈20 cm<sup>-1</sup> of their predicted wavenumber values. In the experimental Raman spectra, there are two intensive bands at 1665 and 1605 cm<sup>-1</sup> that belong to the carbonyl group of the six-membered ring and the C=C group of the same ring. The experimental UV-Vis spectrum of TP was obtained in ethanol between 200 and 450 nm and was theoretically predicted using the Time-Dependent Density Functional Theory (TD-DFT) calculations. Both the experimental and theoretical data show a wide peak at ≈240 nm which suggests that experimental and theoretical data are well-correlated. The solvent effect was explained through the analysis of orbitals and electron density distribution over the polar groups. A high correlation coefficient was also calculated for the experimental and theoretical chemical shifts in the NMR spectrum (0.999). These findings suggest that the B3LYP/6-311++G(d,p) method describes well the experimental results and that it can be used for the determination of TP. This paper can be a starting point for the development of methods for predicting the spectra of newly obtained steroids or similar misused substances.



8-2

### **Spectroscopic and theoretic analysis of hydrocortisone – forensic aspects**

Andjela Gavran, Dusan Dimic

University of Belgrade-Faculty of Physical Chemistry,  
Studentski trg 12-16, 11000 Belgrade, Serbia

Hydrocortisone, or cortisol, is a glucocorticoid secreted by the adrenal gland. Glucocorticoids are a group of steroid hormones important for the daily lives of people. Spectroscopic analysis of hydrocortisone can be beneficial in forensic science and medicine because of the misuse of glucocorticoids in sports. Density functional theory (DFT) was applied as a significant research tool to confirm conclusions obtained in spectroscopic analysis. The theoretical structure of hydrocortisone was optimized at the B3LYP/6-31G(d,p) level of theory, and bond lengths and angles were compared to those of crystallographic structure. The mean absolute error for bond lengths was 0.02 Å, while for bond angles 1.8°. These results suggested that the model reproduced well the experimental structure. DFT was also applied for the prediction of the vibrational (infrared) and electronic (UV-VIS) spectra of hydrocortisone. Assignment of most protruding stretching bands in the theoretical vibrational spectrum showed a small difference when compared to the calculated ones. The most intensive bands were positioned at 1672 and 1707 cm<sup>-1</sup> and belong to stretching vibrations of the two carbonyl groups. In the experimental IR spectrum, positions of the bands corresponding to the carbonyl groups were recorded at 1643 cm<sup>-1</sup> and 1707 cm<sup>-1</sup>, respectively. Small deviations in positions of bands could've been a result of optimization in a vacuum since there are no interactions between molecules as in the KBr pellet. The electronic spectrum was predicted using a Time Dependent-Self Consistent Field (TD-SCF) method. A large number of electronic transitions were in the area obtained experimentally because excited orbitals have similar energies. The most intense transition was positioned at 232,07 nm and the value was close to the experimental position at 241,76 nm. The difference is probably because of the intermolecular interactions with water molecules. These results indicated that DFT methods can be applied for the prediction of spectra that could help in identifying misused substances.

8-3

### The role of defects in graphene for removal of toxic compounds – Theoretical analysis

Marko Jelić<sup>1,2</sup>, Aleksandar Jovanović<sup>1</sup>, Igor Pašti<sup>1</sup>

<sup>1</sup>*Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia,*

<sup>2</sup>*Laboratory of Physics, Vinča Institute of Nuclear Sciences – National Institute  
of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*

Understanding the adsorption of pesticides and toxic gases on graphene has high importance for their degradation and removal. In the present study, the adsorption of different models of organophosphate pesticides (OPH3, OPF3, SPH3 and SPF3) and inorganic molecules (H<sub>2</sub>O and NH<sub>3</sub>) on perfect and defected graphene was examined by using the DFT method. Inspected systems were pristine, single-vacancy (SV), Stone-Wales (SW) and epoxy graphene. Pristine graphene exhibits great adsorption affinity towards OPH<sub>3</sub> molecule, while it shows insignificant adsorption towards other examined species. The introduction of defects influences the reactivity of these molecules on the graphene surface. Among them, SV graphene showed the highest adsorption affinity for H<sub>2</sub>O, NH<sub>3</sub>, OPH<sub>3</sub> and OPF<sub>3</sub>, while SW graphene showed the most suitable adsorption properties towards SPH<sub>3</sub> and SPF<sub>3</sub> molecules. The interaction between molecules and graphene was mostly physisorption except in the case of epoxy graphene where degradation of organophosphates occurred (Figure 1). This study suggests that graphene can be potentially used to remove environmental pollutants and pesticides' chemical degradation, while the surface chemistry of graphene should be carefully tailored for this application.

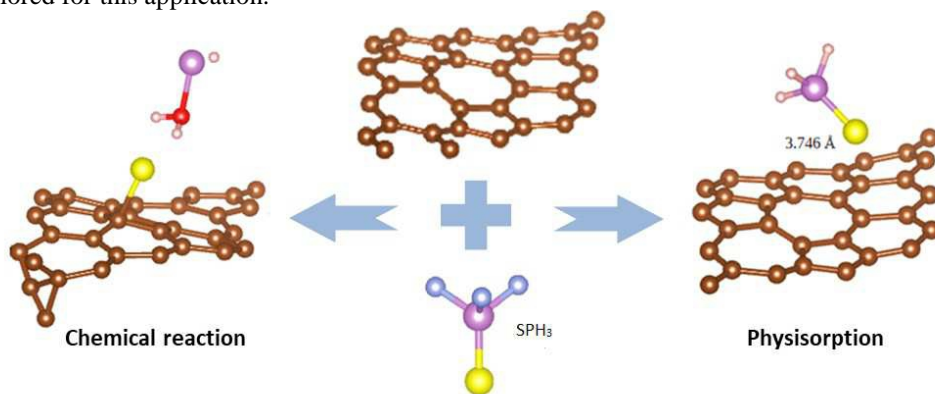


Figure 1. Schematic representation of the interaction between SPH<sub>3</sub> molecule and the graphene

8-4

**A DFT study of the influence of chemical environment and boron concentration in boron-doped graphene on its reactivity**

Milica S. Ritopečki, Ana S. Dobrota

*University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia*

In the past decade, a lot of effort has been focused on constructing and utilizing graphene-based materials for energy-related applications. Functionalization and doping of pristine graphene by boron change its physical and chemical properties, which makes it suitable for new uses. For these reasons, a DFT (Density Functional Theory) study of Al and Na interaction with pristine and doped graphene, both non-functionalized and functionalized with oxygen or hydroxyl group, has been performed. Depending on the concentration of boron, doped graphene has showed increased affinity toward tested metals compared to pristine graphene. Furthermore, increasing the concentration of boron, the presence of functional groups influenced the reactivity of graphene basal plane with metals in a complex manner – in some instances increasing and in some decreasing the reactivity. In certain cases, hydroxide formation would occur, making an irreversible change unsuitable for energy uses.

8-5

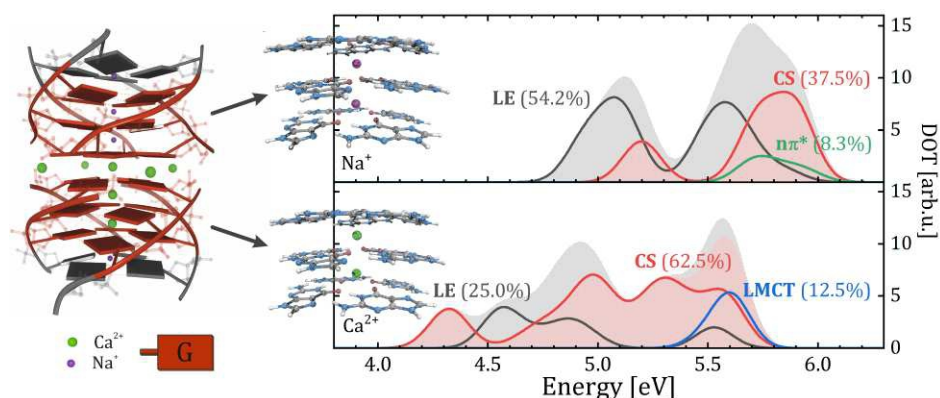
# **Significant modulation of charge-transfer states properties in the biological assembly of the d(TG<sub>4</sub>T) sequence in crystal form**

Branislav Milovanović<sup>1</sup>, Milena Petković<sup>1</sup>, Mihajlo Etinski<sup>1</sup>

<sup>1</sup>University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia

Nucleobase self-assemblies are promising candidates as supramolecular platforms for potential optoelectronic applications. Guanine (G) and its derivatives can self-assemble into so called G-quartets (G4) which could further stack into columnar aggregates [G-octets (G4), G-quadruplexes (GQ)]. These aggregates can accommodate cations between consecutive G4 layers which are very important from the aspect of the stability. These cations can also be used to tune their ground and excited state properties. It is previously showed that alkaline cations cannot modulate electronic absorption spectrum of G8 structures. On the other hand, there are indications that divalent cations such as Mg<sup>2+</sup> and Ca<sup>2+</sup> could be able to modulate excited charge-transfer states of G8.<sup>[1]</sup> Here we report extension to our previous study<sup>[1]</sup> by investigating charge-transfer properties of the crystal structure of a DNA GQ sequence, d(TG<sub>4</sub>T), crystallized in the presence of Na<sup>+</sup> and Ca<sup>2+</sup> ions. In this crystal form Na<sup>+</sup> and Ca<sup>2+</sup> are sandwiched between every G4 layer within GQ central cavity. Excited states analysis (Fig. 1) suggests significant differences between GQ-Na<sup>+</sup> and GQ-Ca<sup>2+</sup> density of transitions. GQ-Ca<sup>2+</sup> spectra is redshifted compared to GQ-Na<sup>+</sup> and exhibit almost twice as much of CS states as well as the presence of LMCT states. This example illustrates possible way of tuning excited state properties of GQ systems for potential application in the optoelectronic devices.

*Figure 1. From left to right: examined GQ d(TG<sub>4</sub>T) crystal structure, extracted computational model and decomposed density of transition spectra into local excitation (LE), charge separation (CS), nπ\* and ligand(G) to metal charge transfer (LMCT) contributions.*



[1] Milovanović B., Stanković I., Petković M., Etinski M., J. Phys. Chem. A **2020**, 124, 40, 8101.

9-1

### **Nitrogen-doped graphene nanoribbons: DFT prospects for Al-ion battery application**

Jovana Vlahović<sup>1,2</sup>, Ana S. Dobrota<sup>1</sup>, Natalia V. Skorodumova<sup>3,4</sup>, Igor A. Pašti<sup>1,3</sup>

<sup>1</sup>*University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia,* <sup>2</sup>*University of Belgrade, Vinča Institute of Nuclear Sciences, Laboratory of Physics, Belgrade, Serbia,*

<sup>3</sup>*KTH-Royal Institute of Technology, School of Industrial Engineering and Management, Department of Materials Science and Engineering, Brinellvägen 23, Stockholm, 100 44, Sweden,* <sup>4</sup>*Uppsala University, Department of Physics and Astronomy, Box 516, 751 20 Uppsala, Sweden*

Energy production and storage are in the focus of today's scientific research due to the rising energy needs of the society. One of the most exploited systems are the metal-ion batteries (MIB). The most commonly used metal in commercial MIBs is lithium, but it is necessary to find a replacement due to its toxicity, occurrence of dendritic growth and decreasing amounts of Li in natural sources. In order to increase the current density, it is convenient to use some multivalent metal as electrically active specie, instead of lithium. Aluminum is a good candidate due to its highest theoretical volume capacity which is four times higher than that for Li, trivalence, non-toxicity, low mass, and radius and it is the most abundant element in the Earth's crust so it is present in large quantities. In this contribution we report the results of DFT calculations of the adsorption of Al on the hydrogen saturated graphene nanoribbons (GNR) with different nitrogen defects. We demonstrate that the adsorption energies of Al are favorable due to the existence of nitrogen defects. Nitrogen, due to its electronegativity, attracts electrons from surrounding atoms and causes good adsorption of Al. Depending on the way nitrogen is bonded to the graphene nanoribbon, there is a different charge transfer in the system, which is shown by Bader analysis and analysis of diagrams of the density of electronic states. These results show that the hydrogen saturated GNR with nitrogen defects are promising materials for use in electrodes of the metal-ion batteries and that they can be used for producing new MIB with Al as an electroactive specimen.

9-2

**The possibility of achieving bound states in complex periodic potential  
of the Kronig-Penney type**

Jovana Obradović, Jelena Radovanović, Vitomir Milanović  
*School of Electrical Engineering, University of Belgrade,  
Bulevar kralja Aleksandra 73, 11120 Belgrade, Serbia*

We analyze the energy spectra of a complex periodic rectangular potential, and derive the conditions for the occurrence of bound states in such a system. It is shown that the energy value  $E_i$ , for which the imaginary part of the dispersion relation is equivalent to zero and the modulus of the real part is less than one, represents an allowed state, which is doubly degenerate. Solutions of the dispersion relation are discussed in terms of varying the parameters of the structure, such as wells and barriers widths, as well as the complex part of the potential (both in the barrier and the well region). The real-valued parameters, such as wells and barriers widths and effective masses are taken from realistic semiconductor heterostructure systems, including the real parts of the barrier potential.

9-3

**Comparison of numerical methods for solving the effective mass Schrödinger equation for multilayer heterostructure applications**

Novak Stanojević, Jelena Radovanović, Vitomir Milanović  
*School of Electrical Engineering, University of Belgrade,  
Bulevar kralja Aleksandra 73, 11120 Belgrade, Serbia*

Many applications of low-dimensional semiconductor structures require highly accurate solving of one-dimensional effective-mass Schrödinger equation for bound state energies and wavefunctions. In particular, in case of sophisticated multibarrier quantum well (QW) systems such as quantum cascade lasers, small changes in layer thicknesses already lead to significant modification of wavefunctions, which results in altered device properties. Therefore, in order to perform meaningful simulations of complex quantum-well based devices, it is important to start from accurately evaluated energies and wavefunctions.

In this work we analyze the case of an asymmetric quantum well intended for resonant second harmonic generation (SHG), taking into account the position-dependent effective mass. The well layer consists of GaAs while the step and barrier layers were made of the  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  alloy. It is known that for resonant SHG three equidistant states are needed, and the intersubband second-order susceptibility is proportional to the cyclic product of the three dipole matrix elements. By varying the parameters of the QW, that is the dimension of the well and step layers, and the compositions of the step and barrier layer alloys, a suitable QW was chosen with three equidistant states with the energy difference between adjoining states being 116meV. For the selected structure the product of the three dipole matrix elements was found by using different numerical approaches. In the first case, energies are found by solving the derived transcendental equation, while the wavefunctions are calculated using analytic expressions. It was shown that for this calculation method the product of the matrix elements has negligible numerical dependence on the choice of the z-coordinate origin (considering three situations in which the origin was located at different positions in the QW). In the second approach the shooting method was used to determine the bound state energies and wavefunction, and the relevant product of matrix elements. Finally the obtained results were compared with the outcomes of transfer matrix method calculations.

9-4

**Construction of Symmetry-adapted k.p Hamiltonians  
for semiconductor nanostructures**

Milan Jocić, Nenad Vukmirović

*Institute of Physics Belgrade, University of Belgrade,  
Pregrevica 118, 11080 Belgrade, Serbia*

Using ab-initio methods like DFT for nanostructures is computationally very expensive, even with modern supercomputers. However, we will show that an accurate quantitative picture can be obtained with a k.p method by starting with Kohn-Sham (KS) states obtained from ab-initio calculations for bulk structure. We demonstrate this by comparing k.p with DFT calculations for the case of CdSe quantum wells. We obtain the analytical form and numerical parameters of well-studied 4x4 and 8x8 k.p Hamiltonians found in literature, for the case where spin-orbit coupling is omitted and included, respectively. Also, we demonstrate an improvement over 4x4 and 8x8 Hamiltonians, by expanding the number of states from 4(8) to 13(26), which yields more accurate excited states. Another improvement can be made, by using the GW approximation within the many-body perturbation theory, thus correcting the DFT electronic structure. This method can give more accurate bulk band gaps, which in turn yields improved results for nanostructures.



9-5

### **Application of nanomaterials in mechanical engineering**

Dorđe Jovanović<sup>1</sup>, Mladen Krstić<sup>2</sup>, Branislav Milenković<sup>3</sup>

<sup>1</sup>*Mathematical institute of SASA, Kneza Mihaila 36, 11000, Belgrade, Department of Computer Science,* <sup>2</sup>*Faculty of Mechanical and Civil Engineering, Dositejeva 19, 36000, Kraljevo, Department of Mechanical Engineering, Faculty of Applied Science, Dušana Popovića 22a, 18000, Niš, Department of Mechanical Engineering*

Nanotechnology is a science about small things, things that are the size measured in nanometers. It is a science that focuses on studying nanomaterials and by that it studies creating and manipulating the elements that are not visible by the naked eye. It is possible to do minor changes in the structure of the elements or materials, thus changing their original characteristics by which they are described. Those new materials represent an evolutionary progress of all aspects of today's science. Theoretically, it is possible to wipe out all diseases, prolong our life expectancy, create new types of foods and drinks and even create new types of clothing by enhancing the materials from which they are made of. All of that is possible because of the new type of manufacturing and manipulating materials on a nanometer scale. Opposed to theory, practice shows that the industry is not yet ready for that kind of progress since there are no materials developed that could manipulate matter on such a small scale. The other problem is the economic profitability of particular processes credited for obtaining new materials with better characteristics.

9-6

### **Numerical study of coupled heat and moisture transfer in a finite wall: effect of wall material on transfer properties**

Zahreddine Hafsi

*Laboratory of Applied Fluids Mechanics Process and Environment Engineering,  
National Engineering School of Sfax, University of Sfax, Sfax 3038, Tunisia*

In this work, a numerical study is conducted for characterization of a wall made up of a bio-based material. Evolutions of hygrothermal properties of the material were followed up in order to judge about the reliability of the material in terms of hygric and thermal insulation. Obtained numerical results were compared to experimental ones issued from previous literature works in order to validate the numerical model. The model was built using COMSOL Multiphysics software. Thus, the “Heat and Moisture Transport” module that couples both sub-modules of heat transfer and moisture transport in building materials was utilized. Comparison of numerical results to experimental ones has proven the efficiency of the numerical model. Then, the study was extended to test other samples of building materials of various compositions put under different hygric and thermal conditions.

10-1

**Simply prepared Mg-V-O as potential cathode material  
for rechargeable aqueous magnesium ion batteries**

Milica M. Vasić<sup>1</sup>, Miloš Milović<sup>2</sup>, Danica Bajuk Bogdanović<sup>1</sup>, Milica Vujković<sup>1</sup>

<sup>1</sup>*University of Belgrade - Faculty of Physical Chemistry, Belgrade, Serbia,*

<sup>2</sup>*Institute of Technical Sciences of SASA, Belgrade, Serbia*

Although today widely used in electronic devices and electric vehicles, lithium ion batteries encounter problem of future application, resulting from limited Li resources, relatively high costs and operational safety problems. Rechargeable magnesium batteries as a potential alternative to the Li-ion ones stand out because of their high theoretical specific capacity, high abundance of Mg resources, atmospheric stability, safety of handling, eco friendliness and low cost. Layered materials including oxides, sulphides and selenides are promising candidates for host materials for Mg<sup>2+</sup> storage in rechargeable magnesium batteries.

Slow migration of Mg<sup>2+</sup> in the layered oxides, ascribed to the strong interaction between Mg and neighbouring O atoms, inspires researchers to look for the ways of improving their electrochemical performance. In this work, Mg-V-O material was synthesized by simple precipitation method, followed by thermal annealing. The obtained material is single-phase material consisted of MgV<sub>2</sub>O<sub>6</sub> phase, according to the results of XRD, FTIR and Raman spectroscopy. Electrochemical test by cyclic voltammetry in aqueous solution revealed redox peaks corresponding to the insertion/deinsertion of Mg<sup>2+</sup> ions into/from the material, but with poor current densities. In order to improve the electrochemical performance of the simply prepared Mg-V-O material, carbon was integrated with the Mg-V-O by sucrose-assisted thermal treatment. Although composed of several phases, the obtained Mg-V-O/C material exhibited around 40 times higher maximal specific current values of Mg<sup>2+</sup> insertion/deinsertion than the Mg-V-O. Also, the electrochemical performance of the Mg-V-O/C for the insertion/deinsertion of Mg<sup>2+</sup> ions was better than those of Al<sup>3+</sup> and Li<sup>+</sup> ions.

Acknowledgements: This research was supported by the Science Fund of the Republic of Serbia, under the project PROMIS #6062667 (HISUPERBAT).

10-2

### **Layered $\text{CaV}_2\text{O}_6$ as promising electrode material for multivalent storage**

Tamara Petrović<sup>1</sup>, Miloš Milović<sup>2</sup>, Danica Bajuk-Bogdanović<sup>1</sup>, Milica Vujković<sup>1</sup>

<sup>1</sup>*Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia,*

<sup>2</sup>*Institute of Technical Sciences of SASA, Belgrade, Serbia*

While the world is facing a higher demand for lithium, its limited resources associated with the high price, are becoming problematic. Other crucial drawbacks of Li-ion batteries are their toxicity and safety concerns. Therefore, researchers are oriented towards development of non-Li batteries based on eco-friendly and earth-abundant materials to overcome drawbacks of Li-ion technology. Alternative abundant metals and their ions such as Mg and Ca could be a good choice for rechargeable batteries in terms of cost and eco-friendliness.  $\text{Mg}^{2+}$  and  $\text{Ca}^{2+}$  ions could transfer two electrons per redox process which theoretically has a positive effect on battery performance. The materials upon which multivalent ions will intercalate with fast diffusion rate are hard to find. Metal vanadium oxide ( $\text{M}_x\text{V}_y\text{O}_z$ ) materials become promising materials for rechargeable batteries, so herein, a standard sol-gel combustion route was used for the preparation of the  $\text{CaV}_2\text{O}_6$  layered precursor. Two samples are synthesized from the vanadate precursor, the first when it was heated at 400 °C ( $\text{CaVO}$ ) and the second when  $\text{CaVO}$  was integrated with 10 wt % of sucrose under thermal treatment at 400 °C, in Ar atmosphere ( $\text{CaVO/C}$ ). Obtained  $\text{CaVO}$  and  $\text{CaVO/C}$  powders were thoroughly characterized by XRD, TG-DTA, FTIR, and Raman spectroscopy. The electrochemical performance of the obtained samples was evaluated for multivalent-ion storage in saturated aqueous electrolytic solutions of Mg ( $\text{NO}_3$ )<sub>2</sub> and Ca ( $\text{NO}_3$ )<sub>2</sub> by cyclic voltammetry and chronopotentiometry. For comparison, measurements were also done in saturated  $\text{LiNO}_3$ . Results indicated that  $\text{CaVO}$  can store more  $\text{Li}^+$  ions than  $\text{Mg}^{2+}$  and  $\text{Ca}^{2+}$  ions, but  $\text{CaVO}$  in  $\text{LiNO}_3$  shows a substantial loss of capacity upon cycling, which is not observed in the case of Mg ( $\text{NO}_3$ )<sub>2</sub> and Ca ( $\text{NO}_3$ )<sub>2</sub>. On the other hand,  $\text{CaVO/C}$  composite showed a significant improvement for Ca and Mg storage capacity, which exceeded capacity storage of  $\text{Li}^+$  ions. The high and stable discharge capacity of  $\text{CaVO/C}$ , amounting to 89.3 mA h g<sup>-1</sup> at 0.5 A g<sup>-1</sup>, was obtained in Ca ( $\text{NO}_3$ )<sub>2</sub>. Obtained results are promising and open novel directions regarding the use of  $\text{CaV}_2\text{O}_6$  for multivalent rechargeable batteries, especially for Ca-ion batteries.

*Acknowledgment:* This research was supported by the Science Fund of the Republic of Serbia, PROMIS, #6062667, HISUPERBAT.

10-3

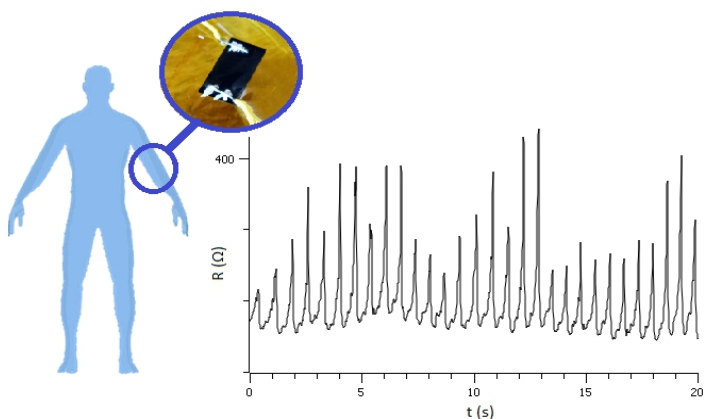
### **Wearable Graphene Sensor for Pulse Measurement**

Teodora Vićentić<sup>1</sup>, Milena Rašljčić Rafajilović<sup>1</sup>, Bojana Koteska<sup>2</sup>,  
Ana Madevska Bogdanova<sup>2</sup>, Igor Pašti<sup>3</sup> and Marko Spasenović<sup>1</sup>

<sup>1</sup>*Center for Microelectronic Technologies, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Serbia,* <sup>2</sup>*Faculty of Computer Science and Engineering, "Ss. Cyril and Methodius" University of Skopje, North Macedonia,* <sup>3</sup>*Faculty of Physical Chemistry, University of Belgrade, Serbia*

Graphene is a material that has been widely used in different types of sensors, due to its optimal electrical and mechanical properties. Recently discovered laser-induced graphene (LIG) has opened new perspectives for a versatile and durable physical sensing platform, capable of detecting various physical parameters.

In this study, LIG was produced by CO<sub>2</sub> laser irradiation of polyimide film. LIG-based sensor was used to measure human pulse. Fabricated LIG sensors were attached to a subject's body, as shown in Figure 1. A temporal change in resistance was recorded for different sensor embodiments, including as-fabricated on polyimide tape and transferred into a PDMS matrix. The measured change in resistance is induced by bending of the sensor due to vein pulsing. The measured resistance time traces were analyzed with the Python HeartPy module to extract pulse information, demonstrating agreement with commercially available sensors.



**Figure 1.** Measuring heart rate with LIG sensor.

We acknowledge support from NATO SPS through project SP4LIFE (G5825).

10-4

**Oxygen sensor based on mechanochemically treated metal oxide  
semiconducting  $\text{TiO}_2\text{-CeO}_2$  mixture**

Jelena N. Stevanović<sup>1</sup>, Srđan Petrović<sup>1</sup>, Dana Vasiljević-Radović<sup>1</sup>,

Katarina Cvetanović<sup>1</sup>, Nenad Tadić<sup>2</sup>, Lazar Rakočević<sup>3</sup>, Milija Sarajlić<sup>1</sup>

<sup>1</sup>*Institute of Chemistry, Technology and Metallurgy, Njegoševa 12, University of Belgrade, Belgrade,* <sup>2</sup>*Faculty of Physics, Cara Dušana 13, University of Belgrade, Belgrade,* <sup>3</sup>*Vinča Institute of Nuclear Science, Mike Petrovića Street 12-14, University of Belgrade, Belgrade*

Simplicity, cost and low energy consumption of a sensor are crucial for integrating into distributed networks of sensor mapping elements for on-site oxygen monitoring in industrial processes, as well as air quality monitoring in environmentally endangered areas. These criteria can be reached with the usage of semiconductor sensors. Despite the high sensitivity, these types of sensors have their drawbacks, such as high operating temperatures, poor selectivity and insufficient long-term stability. The gas sensing performances of the semiconductor sensors could be further advanced to better meet the demands of novel environmental regulations and practical applications via compositing two different metal oxides to form solid solutions or mixtures with separate phases of both constituents. Interface between two oxides was known as the heterojunction, and it refers to modulation of the potential barrier or accumulation layer in the composite.

In this work, we synthesized  $\text{TiO}_2\text{-CeO}_2$  powders by mechanochemical activation in high energy ball mill. Thick films were deposited on alumina substrates with gold electrodes by screen-printing of the paste made out of synthesized composites. Samples were then thermally treated at 800°C. X-ray diffraction (XRD), UV-Visible diffuse reflectance (UV-Vis-DRS), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM) and atomic force microscopy (AFM) were used to evaluate the structural and electronic properties of the prepared materials. The films made of  $\text{TiO}_2\text{-CeO}_2$  were then exposed to various concentrations of  $\text{O}_2$ . The measurements of electrical resistance were performed on 280°C, 300°C and 350°C. With the rising partial pressure of  $\text{O}_2$ , resistance was increasing. It was found that sensitivity of  $\text{TiO}_2\text{-CeO}_2$  composites towards  $\text{O}_2$  strongly depends on working temperature.

10-5

**Improving the electrocatalytic activity of nickel for HER  
in alkaline media by galvanic exchange with rhodium**

Lazar Bijelić, Aleksandar Jovanović, Igor Pašti

*University of Belgrade – Faculty of Physical Chemistry, Belgrade, Serbia*

For the purpose of creating low-cost electrocatalysts for the hydrogen evolution reaction (HER), nickel has gained much attention. This is particularly the case for HER in alkaline media, which, compared to that in acidic media, results in less environmental pollution and equipment corrosion. In the first part of the work, the HER electrocatalytic performance of a rhodium-exchanged smooth nickel disk electrode was studied in a 1 M KOH solution. Rh concentration was varied *via* galvanic exchange of Ni by Rh in a concentrated  $\text{RhCl}_3$  solution for different time intervals. The HER rates measured for the Rh-exchanged Ni electrode were found to be comparable to some of the best-performing electrocatalysts for HER in alkaline media reported so far. The effect of electrode oxidation on the activity of Rh-exchanged Ni disk was also examined and indicated a possible synergistic effect between Ni and Rh. The Ni/Rh ratio of the electrode was measured using energy dispersive X-ray spectroscopy and X-ray photoelectron spectroscopy, latter providing the chemical states of surface atoms as well. A steady increase in Rh concentration with increased exchange time was confirmed. The results from scanning electron microscopy 3D surface reconstruction indicated that there was no substantial change in surface area, indicating an increase of intrinsic catalytic activity upon Ni exchange with Rh. In addition, density functional theory calculations of hydrogen adsorption on the (111) and (100) surfaces of Ni and Rh-exchanged Ni were used to determine the adsorption energies and rationalize an increased HER activity. Based on the lessons learned with smooth Ni model electrodes, in the second part of the work we demonstrated the same approach for boosting HER activity of more realistic, high surface area catalysts – Ni foam and electrodeposited Ni electrodes. In these cases, HER activity is also significantly improved, but the exchange of Ni with Rh seems to be slower. This work demonstrates that the Rh-exchanged Ni electrodes show a high potential as electrocatalysts for HER in alkaline media, with only slightly increased costs compared to that of pure nickel. Acknowledgement: This work was supported by the Science Fund of Republic of Serbia within the project RatioCAT.

10-6

### **Hydrogen evolution on graphene supported PtAu nanoparticles**

Lazar Rakočević<sup>1</sup>, Ivana Stojković-Simatović<sup>2</sup>, Aleksandar Maksić<sup>1</sup>,  
Vladimir Rajić<sup>1</sup>, Svetlana Štrbac<sup>3</sup>, Irina Srejić<sup>1</sup>

<sup>1</sup>INN Vinca, Laboratory of Atomic Physics, University of Belgrade, Serbia, Mike Alasa 12-14, 11001 Belgrade, Serbia, <sup>2</sup>Faculty of Physical Chemistry, University of Belgrade, Serbia, Studentski trg 12-16, 11158 Beograd, Serbia, <sup>3</sup>Institute of Chemistry, Technology and Metallurgy, Department of Electrochemistry, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia

Finding suitable catalysts for hydrogen evolution reaction (HER) is key for economic production of hydrogen for use in fuel cells. Reducing the amount of expensive noble metals that are used is one of the ways for obtaining such catalysts. Various combinations of different noble metals and various carbon supports have been studied.

In this work graphene was used as a support and on it Pt and Au nanoparticles were spontaneously deposited in sub monolayer nanoislands. Obtained PtAu/Graphene electrode was characterized by X ray photoelectron spectroscopy (XPS) and scanning electron microscopy (SEM) while its electrocatalytic activity was investigated by cyclic voltammetry (CV), linear sweep voltammetry (LSV) and chronoamperometry. XPS analysis showed that the atomic percentages of Au and Pt in PtAu/Graphene were 0.6% and 0.3%, respectively. The atomic percentage of Au alone on previously prepared Au/Graphene was 0.7%. SEM micrographs of PtAu/Graphene electrode surface showed that Pt nanoparticles occupy both the edges of previously deposited Au nanoparticles and the edges of graphene support. Average size of PtAu nanoislands is estimated between 60nm and 90 nm. PtAu/Graphene electrode has shown remarkably good performance for HER reaction in 0.5 M H<sub>2</sub>SO<sub>4</sub> acid solution. Outstanding HER activity was achieved, showing the initial potential close to the equilibrium potential for HER and a low Tafel slope of -38 mV/dec. The chronoamperometric measurement performed over 40 min for hydrogen evolution at the constant potential indicates good stability and durability.

11-1

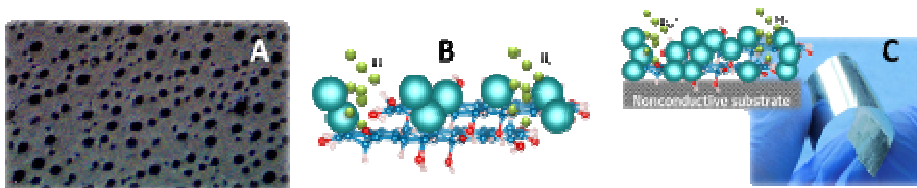
## Electrochemical deposition for advanced engineering of novel electrocatalytic interfaces

Aleksandar Z. Jovanović<sup>1</sup>, Sanjin J. Gutić<sup>2</sup>, Lidija Rafailović<sup>3</sup>, Igor A. Pašti<sup>1</sup>

<sup>1</sup>University of Belgrade – Faculty of Physical Chemistry, Belgrade, Serbia, <sup>2</sup>University of Sarajevo, Faculty of Science, Department of Chemistry, Sarajevo, Bosnia and Herzegovina,

<sup>3</sup>CEST, Centre of Electrochemical Surface Technology, Wr. Neustadt, Austria

The development of novel electrocatalysts requires affordable metals and proper electrode material design from atomic to the macroscopic scale. The electrodeposition makes it possible to develop advanced electrocatalytic materials and surfaces. These either contribute catalytic activity through the increase of electroactive surface or *via* the formation of complex interfaces that increase the rates of electrocatalytic processes. Here we demonstrate three different ways to produce advanced electrocatalytic interfaces. Using hydrogen bubble templating, we have engineered highly developed fcc Ni surfaces with the addition of Co and Fe (Figure, A). These materials possess high catalytic activities for hydrogen evolution reaction (HER) and methanol oxidation. Next, using simultaneous electroreduction of drop-casted graphene-oxide (GO) films on conductive substrates and different metals' electrodeposition, we have made complex metal/reduced GO (Figure, B). These materials have greatly enhanced HER activity, compared to pure electrodeposited metals. Finally, by electrodeposition of Ni onto chemically reduced GO films on the poorly conductive substrate, we produced extended (tens of cm<sup>2</sup>) self-standing porous rGO/Ni foils (Figure, C). These foils can be used as electrocatalysts or current collectors in advanced energy conversion systems. In conclusion, electrodeposition is a simple and scalable approach for the design of superior low-cost electrocatalysts.



This work was supported by the Science Fund of the Republic of Serbia through the project RatioCAT (PROMIS program, ID 606224), and by the COMET program by the Austrian Research Promotion Agency (FFG) and the governments of Lower and Upper Austria.



11-2

**Effect of different cobalt loadings on the electrochemical performance of aluminum pillared clay-supported cobalt towards glucose oxidation**

Biljana Milovanović, Tihana Mudrinić, Sanja Marinović, Marija Ajduković,  
Aleksandra Milutinović-Nikolić, Predrag Banković

*University of Belgrade - Institute of Chemistry, Technology and Metallurgy, National  
Institute of the Republic of Serbia, Department of Catalysis and Chemical Engineering,  
Njegoševa 12, Belgrade, Serbia*

This work is focused on our further efforts to improve the electrochemical performance of cobalt oxide supported on aluminum pillared clay (CoAP) towards glucose oxidation. To this end, the effect of different cobalt loadings onto the electrochemical performance of CoAP was investigated. Four CoAP samples, with theoretical cobalt loadings corresponding to 1, 3, 5, 10 wt% introduced to the pillared clay (x%CoAP), were prepared using the incipient wetness impregnation method. Furthermore, electrodes based on the obtained materials were prepared in the form of carbon paste electrode (CP-x%CoAP) with the same x%CoAP to carbon black (CB) mass ratio. The electrochemical performance of each of CP-x%CoAP was investigated using the cyclic voltammetry in alkaline solution with different glucose concentrations. The electrochemical measurements were carried out in a three-electrode system with an Ag/AgCl and platinum rod as the reference and counter electrodes, respectively. Preliminary results revealed that cobalt content in the pillared clay (AP) significantly affected both the intensity of the current peak of glucose oxidation and sensitivity. It should be emphasized that it was previously shown that CB and AP are not electroactive toward glucose oxidation. The electrode with the lowest cobalt content exhibited the highest current response and the highest sensitivity in the concentration range up to 5 mM. These results indicate that the variation of cobalt content could be used for fine-tuning of the electrocatalytic performance of CP-CoAP. The characterization of the synthesized materials required for establishing the correlation between the physical-chemical properties and the corresponding electrochemical performance of CP-CoAP is ongoing.

11-3

**Synthesis and characterization of new dysprosium doped phosphate-tungsten bronze**

Tijana Maksimović<sup>1</sup>, Jelena Maksimović<sup>2</sup>, Pavle Tančić<sup>3</sup>,  
Ljubinka Joksović<sup>1</sup>, Maja Pagnacco<sup>4</sup>, Zoran Nedić<sup>2</sup>

<sup>1</sup>*Faculty of Science, Department of Chemistry, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac, Serbia,* <sup>2</sup>*Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, 11001 Belgrade, Serbia,* <sup>3</sup>*Geological Survey of Serbia, Rovinjska 12, 11000 Belgrade, Serbia,* <sup>4</sup>*Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia*

Dysprosium phosphate tungsten bronze has been successfully synthesized and characterized (TGA, DSC, FTIR). For the preparation of dysprosium phosphate tungsten bronze (Dy-PWB), as a starting material is used 12-tungstophosphoric heteropoly acid  $\text{H}_3\text{PW}_{12}\text{O}_{40} \times 29\text{H}_2\text{O}$  (PWA), which was first transformed into  $\text{H}_3\text{PW}_{12}\text{O}_{40} \times 6\text{H}_2\text{O}$  (6-PWA) by heating of PWA at 80 °C in a kiln. Aqueous solution  $\text{H}_3\text{PW}_{12}\text{O}_{40} \times 6\text{H}_2\text{O}$  is then commingled with aqueous solution of  $\text{DyCl}_3 \times 6\text{H}_2\text{O}$ , slightly heated in order to start the crystallization process and left during the night to finish the crystallization. The obtained salt  $\text{DyPW}_{12}\text{O}_{40} \times n\text{H}_2\text{O}$  is then heated in furnace, from room temperature to 600 °C, whereby the yellow crystals of dysprosium phosphate tungsten bronze are formed. The structure and its phase transformations were characterized by thermal analysis (TGA and DSC) and Fourier-transform infrared spectra (FTIR).

In this paper, the dysprosium phosphate tungsten bronze has been synthesized and characterized for the first time in order to obtain more information about its structure, chemical features and potential practical application. The potential practical application of Dy-PWB is in its installation in batteries and fuel cells, as catalyst for the reduction of oxygen in acidic electrolytes. Due to the specific yellow color and its thermal stability, Dy-PWB could also be used as a pigment.

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11-4

**Novel PAN-based Air Filters for Potential Applications  
in Industrial Air Filtering and Facemask Production**

Mihailo Mirković<sup>1</sup>, Dušica Stojanović<sup>1</sup>, Daniel Mijailović<sup>2</sup>,  
Nemanja Barać<sup>2</sup>, Đorđe Janačković<sup>1</sup>, Petar Uskoković<sup>1</sup>

<sup>1</sup>*University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120  
Belgrade, Serbia,* <sup>2</sup>*Innovation Center of Faculty of Technology and Metallurgy in Belgrade  
Ltd., Karnegijeva 4, 11120 Belgrade, Serbia*

Air pollution is often related to increased concentration of particulate matter 2.5 (PM<sub>2.5</sub>) pollutant particles in the air. One of the methods of their removal is air filtration. Hereby, a novel and simple method of producing nanofiber-based air filters with multiple active components for highly efficient PM<sub>2.5</sub> capture is proposed. Micro-porous carbon nanofibers (MCNFs) were produced by carbonizing electrospun polyacrylonitrile (PAN) polymer and was later incorporated into the nanofibrous structure of the filters, which itself was made from electrospun PAN, achieving the production of two active components of the filter from one starting material, simplifying the production process. When compared to the base PAN filter, PAN/MCNFs filter exhibits greater filtering properties with almost absolute pollutant particle removal. Their improved thermal and mechanical properties make this kind of filters suitable for harsh-condition environments, such as those in industrial plants. The possibility of using studied filters in facemask production was studied and reduced temperature variation was recorded when using a facemask with an inserted PAN/MCNFs filter, thus increasing wearing comfort for the user. All mentioned properties open a potential possibility for these filters to be used in different environments, but also leave room for further improvement.

11-5

### **High temperature tribological testings of TiAlN coating**

Vladimir Terek<sup>1</sup>, Lazar Kovačević<sup>1</sup>, Aleksandar Miletić<sup>2</sup>,  
Branko Škorić<sup>1</sup>, Aljaž Drnovšek<sup>3</sup>, Zoran Bobić<sup>1</sup>, Pal Terek<sup>1</sup>

<sup>1</sup>*University of Novi Sad, Faculty of Technical Sciences, Department of Production Engineering, Novi Sad, Serbia,* <sup>2</sup>*Polytechnique Montreal, Department of Engineering Physics, Quebec, Canada,* <sup>3</sup>*Jožef Stefan Institute, Department of Thin Films and Surfaces Ljubljana, Slovenia*

Over the last few decades, TiAlN coating has been widely used for various applications at high working temperatures. Apart from coating's mechanical properties, microstructure, and oxidation resistance, tribological behavior is also vital for its successful usage. However, high temperature tribological behavior of coatings can be studied using two methods, directly at high temperatures or on previously annealed samples. This work aims to show the difference between these two testing methods. In this study, 3  $\mu\text{m}$  thick TiAlN coating (3050 HV<sub>0.05</sub>), deposited on hot-working tool steel (EN X38CrMoV5) using cathodic arc deposition, was tested on high temperature pin-on-disk tribometer. Tribological tests were conducted in air atmosphere, against Al<sub>2</sub>O<sub>3</sub> ball, at room temperature (RT), 300, 500, 600 and 700 °C and on samples annealed (AN) at the same temperatures. After tribo-tests, wear tracks were characterized using confocal microscopy, stylus profilometry, focused ion beam and energy dispersive spectroscopy. Tribological tests at RT and on AN samples showed quite similar values of steady-state coefficient of friction (COF), but each of the AN tests displayed pronounced oscillations of COF. At high temperatures COF values increased with increase in number of cycles. However, for tribological tests at 600 and 700 °C decrease of COF was observed after a certain number of cycles. Wear tracks at RT and on AN samples displayed both abrasive and adhesive wear mechanism, while abrasive and oxidative wear mechanisms were observed at high temperatures. Oxidation of substrate material through micro-cracks inside of wear track initiated degradation and completely damaged the coating at 600 and 700 °C, respectively. Therefore, it is suggested that decrease of COF values at 600 and 700 °C is a result of formation of Fe-O and Cr-O inside of wear tracks during tribo-tests. Additionally, it was found that wear rate of coating at RT and on AN samples is quite similar, while high temperature tribo-tests displayed significantly lower wear rates. Finally, it was concluded that tribological tests performed on AN samples are significantly different than high temperature tests but very similar to tests at RT and therefore not adequate for simplifying the high temperature tribological investigations.

11-6

**Effects of corrosion on NiTi caused by fluoride  
and chloride media in non-accelerated corrosion tests**

Zoran Bobić<sup>1</sup>, Bojan Petrović<sup>2</sup>, Sanja Kojić<sup>1</sup>, Vladimir Terek<sup>1</sup>,  
Lazar Kovačević<sup>1</sup>, Goran Stojanović<sup>1</sup>, Branko Škorić<sup>1</sup>, Pal Terek<sup>1</sup>

<sup>1</sup>*University of Novi Sad, Faculty of Technical Sciences, Department of production  
Engineering, Novi Sad, Serbia,* <sup>2</sup>*University of Novi Sad, Faculty of Medicine, Novi Sad,  
Serbia*

Nitinol is an alloy that is widely used in orthodontic applications due to its special mechanical properties and biocompatibility. During application, orthodontic wires are exposed to fluoride and chloride environments that cause decrease of corrosion resistance of NiTi. In previous investigations from literature the effects of corrosion were intensified by using very aggressive media, due to simplified characterization. Consequently, previous results do not sufficiently resemble a real situation. Therefore this study aimed to evaluate the effects of corrosion on predefined location in non-accelerated corrosion tests by observing the changes in surface topography and chemical composition. In this study, we examined the behavior of NiTi (60% Ni and 40% Ti) exposed to different media for 21.5 days: specimen 1 was exposed to artificial saliva, specimen 2 was exposed to medium with 0.05% sodium fluoride and specimen 3 was exposed to medium with 0.5% chlorobutanol. The corrosion was characterized by observing changes in surface topography. For this purpose, atomic force microscopy (AFM) and scanning electron microscopy (SEM) were employed. AFM and SEM measurements for all specimen were performed on 5 predefined locations of 80 µm area. For the analysis of topographic images, extraction of 10 µm area from 80 µm area, and the calculation of surface roughness parameters (Sa and S10z) image analysis software (SPIP) was used. Paired T-test and ANOVA were used for statistical analysis. For all specimens changes in the surface after the corrosion tests were not noticeable in AFM and SEM images of 80 µm areas. Also, statistical analysis revealed that all medium causes an insignificant change in surface roughness parameters. However, changes in surface topography (AFM) were identified for the 10 µm area only for specimens 2 and 3. Results of paired T-test revealed that only treatments of specimens 2 and 3 cause a significant increase and decrease of Sa and S10z parameters respectively. Results of ANOVA revealed that there is a significant difference between all treatments. These results imply that fluoride and chloride containing media in nonaccelerated corrosion tests cause effects of corrosion on a nano level and that fluoride and chloride medium differently change the surface topography.

12-1

### **Raman Spectroscopy of Quasi-two-dimensional transition metal trihalides**

S. Djurdjić Mijin<sup>1</sup>, AM Milinda Abeykoon<sup>2</sup>, A. Solajić<sup>1</sup>, A. Milosavljević<sup>1</sup>, J. Pešić<sup>1</sup>, M. Šćepanović<sup>1</sup>, Y. Liu<sup>3</sup>, A. Baum<sup>4,5</sup>, C. Petrović<sup>3</sup>, N. Lazarević<sup>1</sup>, Z. V Popović<sup>1,6</sup>

<sup>1</sup>*Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia,* <sup>2</sup>*National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, New York 11973,* <sup>3</sup>*Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973-5000, United States,* <sup>4</sup>*Walther Meissner Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany,* <sup>5</sup>*Fakultät für Physik E23, Technische Universität München, 85748 Garching, Germany,* <sup>6</sup>*Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000 Belgrade, Serbia*

Theoretically speaking, the restriction of only one dimension in a three-dimensional material could result in its layered quasi-two-dimensional (2D) analog which has completely unpredictable properties and therefore hosts various unexpected physical phenomena. Successful exfoliation of quasi-2D grapheme by A. Geim's group in 2004 did not only confirm these expectations and create a platform for experimental investigation of low-dimensional phenomena, but also paved the way for the next-generation nanoelectronic devices. All of the above mentioned strongly contributed to the extensive research on the fundamental properties of quasi-2D materials. Great effort has been put towards realization of a magnetic atomically thin crystals which would open up the opportunities of exploring, or even exploiting, of different 2D magnetic states, expand the scope of their possible applications, and point to the possible emergence of a new quantum state of matter. That being said, it is not surprising that the experimental confirmation of 2D magnetism in transition-metal-trihalides (TMTs) caused a stir in scientific community. In an effort to better understand fundamental properties of these materials we have performed the Raman Spectroscopy Study of the two TMT members – CrI<sub>3</sub> and VI<sub>3</sub>, both of which have been confirmed to host low-dimensional magnetism. This experimental technique was used to probe a reported phase transition in CrI<sub>3</sub> and crystal structure of VI<sub>3</sub>. The phase transition, which transforms the low-temperature  $R\bar{3}$  structure into the high-temperature C2/m structure, with potential co-existence, has been observed at 220 K. Our findings confirm the mentioned phase transition but at much lower temperature of 180 K, and no co-existence has been tracked. Our investigation into the crystal structure of VI<sub>3</sub> tried to give an answer to the long unsolved mystery whether at room temperatures VI<sub>3</sub> crystallizes into a  $P3\bar{1}c$ ,  $R\bar{3}$  or C2/m crystal structure. Interestingly, what we have observed points to the coexistence of short-range ordered  $P3\bar{1}c$  and long-range ordered  $R\bar{3}$  phases.

12-2

### **Finishing of polyamide fabric with some boron compounds**

Milena Nikodijević, Čedomir Dimić, Ivana Petrović, Dragan Đorđević  
*Faculty of Technology, University of Niš*

This paper described finding the most suitable methods of pretreatment polyamide fabric with some boron compounds. It is about finishing processes of polyamide fabric in order to improve capillarity, water absorption, flammability and wetting time. Huge amounts of water, chemicals, dyes and auxiliaries are used in textile finishing processes, which can cause danger to the environment and have a toxic effect on workers in the industry. Therefore, the possibilities to replace harmful chemicals with less aggressive and biodegradable ones have been intensively researched for many years. Depending on the applied more suitable means and their ability to react with the fiber, different properties of the fabric are achieved and aesthetic and exploitation values are increased. The functionality of boron compounds, such as boric acid and its alkyl or aryl substituents (boric acid), borax and sodium tetraborate as antibacterial agents, has been extensively studied in various industries. The research determined that after treatment with boric acid and sodium tetraborate, the hydrophilicity of the fabric increased. Also, there is an increase in water absorption, ie. capillarity and water absorption as well as much faster wetting. When testing the flammability of the fabric, it is noticeable that the raw fabric is difficult to burn and burn, given the presence of auxiliary substances that are applied to the textile during production. By washing and removing these substances, polyamide fabrics become more combustible, ie. constantly burning until complete combustion of whole samples. Polyamide fabric treated with boron compounds begins to burn with self-extinguishing after a few seconds. The obtained results suggest the possibility of using boric acid and sodium tetraborate in the finishing processes of polyamide fabric, all in favor of better effects, savings and environmental protection.

12-3

**Zeolite-containing photocatalysts immobilized on aluminum support by plasma electrolytic oxidation**

Kristina Mojsilović<sup>1</sup>, Nikola Božović<sup>1,2</sup>, Srna Stojanović<sup>3</sup>,

Ljiljana Damjanović-Vasilić<sup>3</sup>, Maria Serdechnova<sup>4</sup>, Carsten Blawert<sup>4</sup>,

Mikhail L. Zheludkevich<sup>4,5</sup>, Stevan Stojadinović<sup>1</sup>, Rastko Vasilić<sup>1</sup>

<sup>1</sup>*Faculty of Physics, University Of Belgrade, Studentski trg 12-16, Belgrade 11000, Serbia,*

<sup>2</sup>*Directorate of Measures and Precious Metals, Mike Alasa 14, Belgrade 11000, Serbia,*

<sup>3</sup>*Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, Belgrade 11000, Serbia,* <sup>4</sup>*Institute of Surface Science, Hemholtz-Zentrum Hereon, Max-Planck-Straße 1, Geesthacht 21502, Germany,* <sup>5</sup>*Institute of Materials Science, Faculty of Engineering, Kiel University, Kaiserstraße 2, Kiel 24143, Germany*

To enhance the efficiency of presently used photocatalytic wastewater cleaning systems significant efforts have been directed towards the synthesis of composite photocatalysts, where plasma electrolytic oxidation (PEO) proved to be an appropriate preparation technique for production of stable oxide coatings. We employed PEO of aluminum in silicate-based electrolyte for creating oxide coatings with immobilized pure and Ce-exchanged zeolites clinoptilolite and 13X. Obtained coatings are characterized for their morphology, phase and chemical composition, photocatalytic activity and anti-corrosion properties. It is observed that all mentioned properties of obtained coatings are dependent on processing time and type of immobilized zeolite. All coatings are partially crystallized containing  $\gamma$ -alumina and aluminosilicate phase sillimanite. Photoluminescence (PL) spectral measurements are utilized as a tool to qualitatively probe Ce content in the coatings and showed that the PL intensity increases with prolonged PEO processing time. Coatings with Ce-exchanged zeolite show higher photocatalytic activity and more effective corrosion protection than those with pure zeolite. The highest photocatalytic activity is detected for coatings obtained through a pulsed DC during 30 min, containing Ce-exchanged 13X zeolite. The effect of Ce is not too strongly pronounced on anti-corrosion properties due to its low concentration in the coatings but it is still visible. Corrosion observations suggest that coatings containing Ce-exchanged 13X zeolite have the highest corrosion resistance which lapses for longer PEO processing time.



12-4

### **Obtaining of healthcare textiles based on viscose fabric with improved sorption properties**

Matea Korica<sup>1</sup>, Zdenka Peršin<sup>2</sup>, Lidija Fras-Zemljič<sup>2</sup>, Mirjana Kostić<sup>3</sup>

<sup>1</sup>*Innovation Center of Faculty of Technology and Metallurgy, University of Belgrade, Serbia,*

<sup>2</sup>*Institute of Engineering Materials and Design, Faculty of Mechanical Engineering,  
University of Maribor, Slovenia,* <sup>3</sup>*Faculty of Technology and Metallurgy, University of  
Belgrade, Serbia*

The growing demand for better healthcare is a major factor in moving the healthcare textile market towards neoteric products with upgraded properties. Sorption properties are one of the most important properties of healthcare textiles because they affect the removal of excess exudates. Removing excess exudates is very pertinent since they contain nutrients that increase the risk of bacterial growth. The application of viscose in healthcare textiles production has a long tradition owing to its intrinsic properties of biocompatibility, nontoxicity, and bioabsorbability. But, although the sorption properties of viscose are much better than those for similar materials such as modal and lyocell, these properties are not sufficient in the cases when is needed exceptional high absorbent capacity.

In this study, viscose fabric was modified in two different ways: 2,2,6,6-tetramethylpiperidine-1-oxy radical (TEMPO) oxidation and coating with TEMPO oxidized cellulose nanofibrils (TOCN), in order to improve its sorption properties by introducing hydrophilic carboxyl groups. The sorption properties of unmodified, TEMPO oxidized and TOCN coated viscose fabrics were determined by measurements of time needed for establishing equilibrium state of absorption, absorbent capacity, and contact angle. Compared to unmodified, TEMPO oxidized and TOCN coated viscose fabrics showed improved sorption properties (increased absorption capacity up to 130 mg liquid/g fabric, decreased time needed to reach equilibrium state from 144 s to 24.7 s and contact angle from 81° to 40°) and may find application as healthcare textiles with upgraded removal of excess exudates.

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12-5

### **Lattice dynamics and magnetism in $\text{Fe}_{3-x}\text{GeTe}_2$**

Ana Milosavljević<sup>1</sup>, Andrijana Šolajić<sup>1</sup>, Sanja Đurđić Mijin<sup>1</sup>, Jelena Pešić<sup>1</sup>,  
Bojana Višić<sup>1</sup>, Yu Liu<sup>2</sup>, Cedomir Petrovic<sup>2</sup>, Zoran V. Popović<sup>1,3</sup>, Nenad Lazarević<sup>1</sup>  
<sup>1</sup>*Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia,* <sup>2</sup>*Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973-5000, USA,* <sup>3</sup>*Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000 Belgrade, Serbia*

$\text{Fe}_{3-x}\text{GeTe}_2$  belongs to a highly experimentally and theoretically studied class of van der Waals ferromagnetic materials. Due to the weak interaction between the layers, the exfoliation of the bulk crystals to mono and a few layers is relatively easy. The magnetic properties of these materials are kept even in a low-dimensional regime which makes this class suitable for possible applications in new device engineering.

$\text{Fe}_{3-x}\text{GeTe}_2$  has a relatively high magnetic transition temperature (220-230 K). This temperature, as well as lattice parameters, strongly depends on vacancies concentration in the sample. Samples with a higher concentration of vacancies grown by flux method have lower  $T_C$  (150 K).

In Raman spectra of flux-grown  $\text{Fe}_{3-x}\text{GeTe}_2$  single crystal four out of eight modes predicted by symmetry are detected ( $2A_{1g} + 2E_{2g}$ ). The experimentally obtained phonon energies are in a good agreement with theoretically calculated values. Temperature dependence of phonon self-energies displays deviation from the conventional model at temperatures around 150 K and 220 K. In addition, at the same temperatures nonmonotonic behavior of electronic continuum is present. While the temperature of the first anomaly coincides with the magnetic phase transition temperature, the anomaly at 220 K remains an open question although can be related to a persistence of short-range magnetic ordering in this compound.

12-6

### **Design of a pump for shipping crude oil from an oil terminal in Cameroon**

Lotin Thierry, Bella Marie

*University of Douala, Faculty of sciences P.O. Box 245 Douala, Cameroon*

This work involves a fluid mechanics study of a centrifugal pump that is intended to ship hydrocarbons to buying vessels to enable them to acquire the hydrocarbons produced from the Republic of Chad in a reliable manner. The necessary parameters that lead to the choice of a pump are the efficiency, the head and the power of the pump. The pump we have designed, which operates at a precise flow rate, will not suffer from cavitation, and furthermore allows the pump's flow rate to be boosted in order to reduce long waiting times. The characteristics of this pump show that: (i) the power versus volume flow curves between the laboratory and on site show a remarkable agreement, reflecting a performance without pressure loss between the different stages. (ii) The efficiency versus flow curves, with some small differences, show the same characteristics in terms of laboratory and field data, which also indicates good performance. The  $NPSH_{dispo}$  value that allowed us to assess the risk of pump cavitation is above 0.5. In the same sense, we verified the relationship:  $NPSH_{dispo} - NPSH_{required} > Tv$  with  $Tv = 0.013$  bar at  $20^{\circ}C$ . All this leads us to say that the pump respects the safety margin. Therefore, it will not cavitate with this operating flow rate, which is approximately  $88 \text{ m}^3/\text{h}$ . Comparisons with the ordinary pumps installed in the various oil tankers in the port of Kribi show that our pump allows the tanks to be filled two to three times faster and saves a considerable amount of time waiting in the port.

13-1

### **Application of supercritical carbon dioxide for making perovskite photodiode**

Milica Stefanović<sup>1</sup>, Rada Petrović<sup>2</sup>, Ivana Lukić<sup>2</sup>, Jelena Vujančević<sup>3</sup>, Đorđe Janačković<sup>2</sup>

<sup>1</sup>*University of Belgrade, Innovation Center of Faculty of Technology and Metallurgy, Belgrade, Serbia,* <sup>2</sup>*University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia,* <sup>3</sup>*Institute of Technical Sciences of SASA, Belgrade, Serbia*

Perovskite solar cells reached high efficiency in a short period. When perovskite was applied for the first time as photovoltaics, power conversion efficiency (PCE) was less than 3 %. Up to now, PCE is over 29 %. In perovskite solar cells, the perovskite layer is an active layer that absorbs the visible part of the spectrum. To reduce the recombination of charge carriers, the construction of solar cells requires the existence of layers for holes and electrons. TiO<sub>2</sub> is usually used as an inorganic electron transport layer because its conduction band (CB) lies under the CB of perovskite, so electrons could diffuse from CB of perovskite to CB of TiO<sub>2</sub>. For these experiments, TiO<sub>2</sub> nanotubular structure was used due to its advantages compared to nanoparticulate TiO<sub>2</sub>. TiO<sub>2</sub> nanotubes provide a one-dimensional transmission channel for the charge carriers which will reduce the recombination of the carriers and provide a fast carrier transport. The TiO<sub>2</sub> nanotubes were synthesized by anodization of Ti foil after which they were annealed at 450 °C for 1 h. Their inner diameter was  $\sim 103 \pm 17$  nm while the length was  $\sim 350$  nm. Methylammonium lead bromide perovskite (MAPbBr<sub>3</sub>) was deposited on TiO<sub>2</sub> nanotubes from the solution in dimethylformamide (DMF) by application of supercritical carbon dioxide at 35 °C and different pressures (100, 200, and 300 bar). It has been observed that supercritical CO<sub>2</sub> improves the filling of nanotubes by the perovskite due to its stronger solubilizing power at higher pressures. A perovskite photodiode with an improved contact surface between TiO<sub>2</sub> and perovskite was made, which is the basis for future solar cell construction. I-V characteristics show that the highest value of photocurrent under visible light reached 400  $\mu$ A for the sample which was obtained at 35 °C and 300 bar for 1 h. The absorption edge of prepared TiO<sub>2</sub> nanotubes/MAPbBr<sub>3</sub>, determined by diffuse reflectance spectroscopy, was extended to the visible range. FESEM and XRD analyses also were done.

13-2

### **Optimisation of materials for enhancement of efficiency of Dye Sensitized Solar Cells**

Evgenija Milinković<sup>1</sup>, Katarina Cvetanović<sup>1</sup>,

Dana Vasiljević-Radović<sup>1</sup> and Dragomir Stanisavljev<sup>2</sup>

<sup>1</sup>*Centre of Microelectronic Technologies, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoseva 12, 11060 Belgrade, Serbia,* <sup>2</sup>*Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, 11060 Belgrade, Serbia*

The world is facing serious issues regarding fossil fuels consumption. As it's known, the remaining quantities of these energy sources are small, and also there is an undesirable effect on the environment. Dye Sensitized Solar cells (DSSC) have vast potential as one of the key solutions in the future due to their easy and unexpensive fabrication and rising energy conversion efficiency.

DSSC is a type of electrochemical system with two electrodes, photoanode and counter electrode, and appropriate electrolyte. The most common photoanode is  $\text{TiO}_2$  anode with dye adsorbed on its surface, while counter electrode and electrolyte are platinum and  $\text{I}^-/\text{I}_3^-$  solution in acetonitrile, respectively. The working principle is based on photoinjection of electrons from dye molecules into a conduction band of  $\text{TiO}_2$  and dye regeneration by  $\text{I}^-/\text{I}_3^-$  redox couple in the electrolyte. Considering the above mentioned, special attention needs to be given to the positions of the energy levels at the electrolyte/dye/oxide interface. Every constituent part of DSSC has an important role in the DSSC functioning, so their optimisation and improvement would lead to the enhancement of the whole system.

In this research, we compared cells fabricated with materials prepared in our lab and cells made with commercial components, all obtained from Solaronix, in order to optimise components and improve procedures for the fabrication of DSSCs. The common component for all cells was commercial  $\text{TiO}_2$  photoanode with reflection layer and N3 dye. We compared electrolyte Iodolyte Z-150 to  $\text{I}^-/\text{I}_3^-$  solution in acetonitrile prepared in our lab, so we can discuss its influence on cells' performances. Also, we prepared cells with two different counter platinum electrodes (one with commercial Platonix T/SP and one with ethanol solution of chloroplatinic acid). All cells were sealed with thermoplastic sealing film (Meltonix foil) that firmly defines the distance between electrodes. Characterization of the manufactured DSSCs has been obtained by linear sweep voltammetry (LSV), open-circuit voltage decay (OCVD), and current transient measurements (CT).

13-3

**Investigation of photo(electro)catalytic efficiency of  $\text{BaTi}_{1-x}\text{Sn}_x$ ,  
 $\text{ZnO}$  and  $\text{ZnO@BaTi}_{1-x}\text{Sn}_x$  ( $x = 0, 0.05, 0.10$ ) powders**

Katarina Aleksić<sup>1</sup>, Ivan Supić<sup>2</sup>, Ivana Stojković Simatović<sup>2</sup>,  
Ana Stanković<sup>1</sup>, Smilja Marković<sup>1</sup>

<sup>1</sup>*Institute of Technical Sciences of SASA, Belgrade, Serbia,*

<sup>2</sup>*Faculty of Physical Chemistry, University of Belgrade, Serbia*

The aim of this research was to improve photo(electro)catalytic properties of  $\text{BaTi}_{1-x}\text{Sn}_x$  (BTS,  $x = 0, 0.05, 0.10$ ) powders. For that purpose we employed ZnO to prepare  $\text{ZnO@BTS}$  composite. *In situ* microwave processing of a ZnO precipitate on previously synthesized BTS particles was used to produce  $\text{ZnO@BTS}$  composites. The phase composition and crystal structure of BTS, ZnO and  $\text{ZnO@BTS}$  were examined by X-ray powder diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR). The powders particles morphology was investigated by field emission scanning electron microscopy (FESEM). The optical properties were studied using UV-Vis diffuse reflectance (DRS) and photoluminescence spectroscopy (PL). Linear voltammetry was used to examine the photoelectrochemical properties of the materials. Photocatalytic properties were tested based on the decolorization of methylene blue (MB) dye in the presence of powder particles, under the influence of simulated sunlight radiation. BTS powders have good electron transfer properties, which has been shown in their function as electrocatalysts, where they have shown better properties than ZnO and  $\text{ZnO@BTS}$  composites. In contrast, they showed poor photocatalytic efficacy. The precipitation of ZnO particles on BTS, by the method of microwave processing, significantly improves the photocatalytic efficiency of the formed composites, concerning the starting BTS powders. Among the composites,  $\text{ZnO@BT}$  composite proved to be the most effective photocatalyst.

13-4

**Thin film nanocomposites based on polyaniline and silver nanowires  
for optoelectronic applications**

Jovan Lukić, Vuk V. Radmilović

*Faculty of Technology and Metallurgy, University of Belgrade, Serbia*

The broad application of optoelectronic devices has influenced intense R&D to follow in its wake. As one of the essential parts of these devices, transparent electrodes (TE) represent an area of growing interest, owing to the fact that it is possible to drastically improve the performance of optoelectronic devices by improving properties of TE.

In this work TE films based on the nanocomposite of silver nanowires (AgNWs) and polyaniline polymer (PANI) were processed via spin coating during which various wt% of polymer dispersions were coated on a layer of AgNWs, after which the nanocomposite was doped with orto-phosphorous acid ( $\text{H}_3\text{PO}_4$ ) in order to transform the polymer from its non-conductive emeraldine base (EB) to its conductive state – emeraldine salt (ES). AgNWs/PANI nanocomposites have shown promising optoelectronic properties, such as optical transparency of 84.6% and sheet resistance of  $35 \Omega/\square$ , essential for adequate TE performance.

13-5

### **Surface phonons in $\text{YVO}_4\text{:Eu}^{3+}$ nanopowders**

**J. Mitrić<sup>1</sup>, N. Paunović<sup>1</sup>, M. Mitrić<sup>3</sup>, J. Ćirković<sup>2</sup>,  
M. Gilić<sup>1</sup>, M. Romčević<sup>1</sup> and N. Romčević<sup>1</sup>**

*<sup>1</sup>Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia, <sup>2</sup>Institute for Multidisciplinary Research, University of Belgrade, Kneza Višeslava 1a, 11030 Belgrade, Serbia, <sup>3</sup>Institute Vinča, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia*

In this work two methods of preparation of yttrium orthovanadate nanopowders were presented: Solid State Reaction (top – down approach) and Solution Combustion Synthesis (bottom – up approach). For starting structural characterization, X – Ray Powder Diffraction (XPRD) and Field Emission Scanning Electron Microscopy (FESEM) were used. We report the change in reflection spectra in europium doped  $\text{YVO}_4$  nanopowders with comparison to its bulk analog. In UV – Vis reflection spectra we consider the change in values of band gap in these structures, after resizing it from bulk to nanomaterial. In Far – Infrared (FIR) reflection spectra, we registered the existence of Surface Optical Phonon (SOP) and different multi – phonon processes which alter the reflection spectra of bulk  $\text{YVO}_4$ . The influence of Eu ions is reflected through multi – phonon processes that occur and are connected with energy transfer from  $\text{YVO}_4$  lattice to Eu ions. All IR spectra were modeled using classical oscillator model with Drude part added which takes into account the free carrier contribution. Since our samples are distinctively inhomogeneous materials, we use Effective Medium theory in Maxwell Garnett approximation to model its effective dielectric function.



13-6

**Hydrothermal synthesis of hydroxyapatite  
on calcium-enriched natural and synthetic zeolite as a carrier**

Katarina Sokić<sup>1</sup>, Đorđe Veljović<sup>1</sup>, Jelena Dikić<sup>2</sup>,

Jovica Stojanović<sup>3</sup>, Danijela Smiljanić<sup>3</sup>, Sanja Jevtić<sup>1</sup>

<sup>1</sup>*Faculty of Technology and Metallurgy, University of Belgrade, Serbia*

<sup>2</sup>*Innovation centre of the Faculty of Technology and Metallurgy, University of Belgrade, Serbia,* <sup>3</sup>*Institute for Technology of Nuclear and Other Mineral Raw Materials, University of Belgrade, Serbia*

The aim of this study was to investigate the possibilities and to optimize the conditions for the synthesis of hydroxyapatite (HAP) on calcium-enriched natural and synthetic zeolites as carriers. Two synthetic zeolites were used in the paper: zeolite 4A (Na-form) and zeolite 5A (Ca-form) as well as natural zeolite - clinoptilolite from Slanci deposit in Serbia. Clinoptilolite and zeolite 4A were enriched with calcium ions by ion exchange treatment in order to enable the source of  $\text{Ca}^{2+}$  in the crystallization of hydroxyapatite. Phosphorus, necessary for the crystallization of hydroxyapatite, was introduced through a solution of ammonium-hydrogenphosphate. The influence of the concentration of hydrogen phosphate ions, temperature and crystallization time of hydroxyapatite on the morphology of the zeolite surface as well as the degree of its coverage with newly formed hydroxyapatite particles was monitored in the experiments. The obtained powders were characterized by X-ray powder diffraction (XRD), thermal TG-DTG analysis, infrared spectroscopy with Fourier transformation (FTIR) and scanning electron microscopy (SEM). Based on the structural analysis, it was shown that the synthesis of hydroxyapatite did not affect on the structure of the zeolite, except in the case when a very concentrated hydrogen-phosphate solution was used. Thermal analysis showed that all obtained zeolite and HAP samples were stable up to 800 °C. Optimization of the hydrothermal crystallization process showed that temperature and time do not have a crucial influence on the synthesis of the materials (similar results were obtained at 120 °C for 20 hours and at 160 °C for 4 hours). When the concentration of the solution of ammonium hydrogen phosphate was higher, larger crystals of hydroxyapatite were obtained, but the crystal lattice of the zeolite was collapsed. SEM micrography showed that unevenly distributed hydroxyapatite crystals were formed on natural zeolite due to the presence of various impurities, while the best results were achieved using zeolite 5A, where the surface of the zeolite is completely covered with crystals of hydroxyapatite.

13-7

**Synthesis of linear and star-shaped oligoimides by high-temperature catalytic polycondensation in a benzoic acid melt according to the Bn + AB scheme**

A.E. Soldatova<sup>1</sup>, A.Ya. Tsegelskaya<sup>1</sup>, I. G. Abramov<sup>2</sup>, A. Kh. Shakhnes<sup>3</sup>,  
O.V. Serushkina<sup>3</sup>, A. Herberg<sup>4</sup>, A.A. Kuznetsov<sup>1</sup>

<sup>1</sup>*Enikolopov Institute of Synthetic Polymeric Materials, Moscow, Russia*

<sup>2</sup>*Yaroslavl State Technical University, Yaroslavl, Russia*

<sup>3</sup>*Zelinsky Institute of Organic Chemistry, Moscow, Russia*

<sup>4</sup>*Paderborn University, Paderborn, Germany*

Aromatic polyimides (PIs) are known as polymers with a unique set of properties. They have excellent mechanical properties, high thermal, chemical and radiation stability. Aromatic PIs are characterized by performance in a wide range of temperatures, from cryogenic to 400°C. They are widely used in various fields, such as aircraft construction, space industry, electrical engineering, electronics, transport engineering etc.

In this work, linear and star-shaped oligoimides were synthesized according to the Bn + AB scheme using a highly efficient, more environmentally friendly and technologically simple method of high-temperature catalytic polycondensation in a benzoic acid melt, where Bn are aromatic amines with the different number of amine groups ( $n = 1, 2, 3$  and  $4$ ), AB - 3-aminophenoxyphthalic acid (APPA). The monomer APPA under the conditions of the process is converted into the amino-anhydride form and becomes monomers of the AB type. In previous studies, star-shaped oligoimides were obtained with slow-addition of AB monomer into the reaction system. In this work, AB monomer was loaded into the reaction system one portion. Also, during the polycondensation of AB monomers, along with the formation of the main products, the formation of cycles occurs. In this work, the effect of loading AB monomer on cyclization was studied, and the first steps were taken to study the mechanism of formation of cycles.

All obtained oligoimides were investigated by IR, <sup>1</sup>H NMR spectroscopy, as well as by the SEC method with triple detection (RI, MALLS and viscosimetry). The process of cyclization by monomer APPA was investigated in more detail using the MALDI ToF method.

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Abramov, I. G.		76
Adamović, Vladimir		23
Ahmetović, Sanita	sanita.ahmetovic@imsi.rs	24
Ajduković, Marija		59
Aleksić, Katarina	katarina.aleksic96@gmail.com	72
Antanasković, Anja	anja.antanaskovic@yahoo.com	23
<b>Bajuk Bogdanović, Danica</b>		<b>36, 37, 38, 39, 52, 53</b>
Banićević, Ivana	ivanaib100@gmail.com	6
Banković, Predrag		59
Barać, Nemanja		61
Baum, A.		64
Bella, Marie		69
Bijelić, Lazar	20170032@student.ffh.bg.ac.rs	56
Blawert, Carsten		66
Blažić, Larisa		11
Bobić, Zoran	zoranbobic@uns.ac.rs	62, 63
Bogosavljević, Marica		34
Bohlen, Jan		10
Božinović, Nevena	nevena.bozinovic@vin.bg.ac.rs	9
Božović, Nikola		66
Branislav, Milovanović	branislavm@ffh.bg.ac.rs	46
Brzić, Saša		34
Budimir, Milica		36
Chernysheva, Anna		40
Chodkowski, Michał	michal.chodkowski@poczta.umcs.lublin.pl	28
Cvetanović, Katarina		55, 71
Cvjetičanin, Nikola		24
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Dimić, Dušan		42, 43
Dimitrijević, Silvana		27
Dimitrijević-Branković, Suzana		12, 14, 25
Dinic, Ivana	ivana.dinic@itn.sanu.ac.rs	29, 33
Dinić, Čedomir		65
Djurdjić Mijin, S.	sanja@ipb.ac.rs	64
Dobrota, Ana S.		45, 47
Dojčinović, Milena	milena.p.dojcinovic@gmail.com	32
Dorontić, Slađana	sladjanaseatovic93@gmail.com	35
Drinić, Zorica		16
Drnovšek, Aljaž		62
<b>Đorđević, Dragan</b>		65
Đorđević, Ivona	djordjevicivo3@gmail.com	19
Đurđić Mijin, Sanja	sanja@ipb.ac.rs	68
<b>Etinski, Mihajlo</b>		46
<b>Fras-Zemljič, Lidija</b>		67
<b>Galić, Aleksa</b>	aleksagalic99@gmail.com	15
Gavran, Andjela	andjela.gavran@gmail.com	43
Gavrilov, Nemanja		38
Gilić, Martina		74
Glojinjić, Marko		38
Grbović Novaković, Jasmina		27
Grozđanić, Nikola		19
Grujičić, Marija	marijagrujicic64@gmail.com	39
Grujić, Bojana	bojana.grujic@aggf.unibl.org	22

Grujić, Dušan		11
Grujić, Žarko		22
Gržetić, Jelena D.	jrusmirovic@tmf.bg.ac.rs	34
Gutić, Sanjin J.		58
Hafsi, Zahreddine	zahreddine.hafsi@enis.tn	51
Herberg, A.		76
Jablonska, Eva		10
Jaćimović, Nevena	nevena.jacimovic.99@gmail.com	7
Janačković, Đorđe		12, 13, 14, 61, 70
Janković, Teodora		16
Jelić, Marko	marko.jelic@vinca.rs	44
Jevtić, Sanja		75
Jocić, Milan	mjocic@ipb.ac.rs	50
Joksović, Ljubinka		60
Jovanović, Aleksandar		44, 56
Jovanović, Aleksandar Z.	a.jovanovic@ffh.bg.ac.rs	58
Jovanović, Đorđe	bmilenkovic92@gmail.com	51
Jovanović, Miloš	mjovanovic@mocbilja.rs	16
Jovanović, Sonja		37, 39
Jovanović, Svetlana		35, 36
Jovanović, Zoran		37, 38, 39
Jurak, M.		3
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Knežević-Jugović, Zorica		20
Kojić, Sanja		63

Korica, Matea	mkorica@tmf.bg.ac.rs	67
Kostić, Marija	mkostic607@gmail.com	1
Kostić, Mirjana		67
Kostjuk, Sergei		40
Koteska, Bojana		54
Kovač, Janez		32
Kovačević, Lazar		62, 63
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Krstić, Jugoslav		32
Krstić, Mladen		51
Kukuruzar, Andrej	andrejkukuruzar.so@gmail.com	26
Kuzmanović, Maja		4
Kuznetsov, A. A.		76
Ładniak, Agata	agata.gozdecka@poczta.umcs.lublin.pl	5
Lainović, Tijana		11
Lazarević, N.		64
Lazarević, Nenad		68
Lazarević-Pašti, Tamara		21
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Liu, Hongzhi		40
Liu, Y.		64
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Lojpur, Vesna		33
Lopičić, Zorica		23
Lotin, Thierry	dipita_lolo@yahoo.com	69
Lukić, Ivana		70
Lukić, Jovan	jovanlukickg@gmail.com	73
Mađevska Bogdanova, Ana		54
Maksić, Aleksandar		57

Maksimović, Jelena		60
Maksimović, Tijana	tijana.maksimovic@pmf.kg.ac.rs	60
Mančić, Lidija		29, 33
Marinković, Dalibor		18
Marinović, Sanja		59
Marković, Olivera		35
Marković, Smilja		16, 32, 72
Matić, Tamara	tmatic@tmf.bg.ac.rs	13, 15
Medić Ilić, Mirjana		27
Mijailović, Daniel		4
Mijatov, Slavko		34
Milanković, Vedran	milankovicvedran@gmail.com	21
Milanović, Igor		27
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Milenković, Branislav		51
Miletić, Aleksandar		62
Miletić, Vesna		13
Milić, Marija		25
Milinda Abeykoon, AM		64
Milinković, Evgenija	evgenija@nanosys.ihtm.bg.ac.rs	71
Milivojević, Marija	mmilivojevic@tmf.bg.ac.rs	12
Milivojević, Milan		23
Milivojević, Milena		6
Milojković, Jelena		23
Milosavljević, A.		64
Milosavljević, Ana	anam@ipb.ac.rs	68
Milovanović, Biljana	biljana.milovanovic@ihtm.bg.ac.rs	59
Milovanović, Dubravka		9
Milović, Miloš		52, 53
Milutinović-Nikolić, Aleksandra		59
Minarik, Peter		10
Mirković, Mihailo	mihailo.mirkovic17@gmail.com	61

Mišković-Stanković, Vesna		30
Mišović, Aleksandra	aleksandra.misovic@vin.bg.ac.rs	36
Mitić Čulafić, Dragana		4
Mitrić, Jelena	jmitric@ipb.ac.rs	74
Mitrić, Miodrag		74
Mladenović, Mihailo	mihailo.mladenovic99@gmail.com	25
Mojović, Miloš		2
Mojsilović, Kristina	kristina.mojsilovic@ff.bg.ac.rs	66
Mravik, Željko	mravik@vin.bg.ac.rs	37, 38, 39
Mroccka, R.		3
Mudrinić, Tihana		59
Nakarada, Đura	djura@ffh.bg.ac.rs	2
Nedić Vasiljević, Bojana		37
Nedić, Zoran		60
Nešović, Katarina		30
Nikodijević, Milena	nikmilena94@gmail.com	65
Nikolic, Marko		29
Nikolić, Maria Vesna		24, 32, 38
Nikolić, Nikolina	nnikolina@vin.bg.ac.rs	31
Novaković, Nikola		27
Novta, Evgenije	evgenije.novta@mf.uns.ac.rs	11
Obradovic, Jovana	jovanaobradovic988@gmail.com	48
Obradović, Bojana		6, 8
Obradović, Nataša		15
Olejniczak, Andrzej		38
Opsenica, Marko	marko.opsenica44@gmail.com	30
Pagnacco, Maja		60
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Pašti, Igor A.		44, 47, 54, 56, 58
Paunović, Novica		74
Pavlović, Marija		6
Pavlović, Stefan	stefan.pavlovic@ihm.bg.ac.rs	18
Pavlović, Vladimir B.		24
Pejčić, Milica	pejcic97m@gmail.com	37
Peršin, Zdenka		67
Pešić, J.		64
Pešić, Jelena		68
Petković, Milena		46
Petrović, Jelena	jelenapetrovic.co@gmail.com	8
Petrović, Bojan		63
Petrović, C.		64
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Petrović, Ivana		65
Petrović, Rada		12, 13, 14, 70
Petrović, Srđan		55
Petrović, Suzana		9
Petrović, Tamara	tamara@ffh.bg.ac.rs	53
Podkościelna, Joanna	terpil@umcs.pl	17
Popović, Miljana		12
Popović, Z. V.		64
Popović, Zoran V.		68
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Rafailović, Lidija		58
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Rakočević, Lazar	lazar.rakocevic@vin.bg.ac.rs	55, 57
Rakočević, Lazar		55
Rašljić Rafajilović, Milena		54
Ristivojević, Nikola	20210324@student.ffh.bg.ac.rs	42
Ritopečki, Milica S.	milica.ritopecki@gmail.com	45
Romčević, Maja		74
Romčević, Nebojša		74
Sarajlić, Milija		55
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Shakhnes, A. Kh.		76
Skorodumova, Natalia V.		47
Smiljanić, Danijela		75
Sokić, Katarina	ksokic@tmf.bg.ac.rs	75
Soldatov, Mikhail	soldat89.89@gmail.com	40
Soldatova, A. E.	soldatova.anastasia92@gmail.com	76
Spasenović, Marko		54
Spasojević, Jelena		31
Spreitzer, Matiaž		32
Srejić, Irina		57
Stamenković, Tijana	tijanas@vinca.rs	33
Stanisavljev, Dragomir		71
Stanković, Ana		72
Stanković, Dalibor		26
Stanković, Miroslav		18
Stanojević, Novak	novakstanojevic1@gmail.com	49
Stefanović, Milica	mstefanovic@tmf.bg.ac.rs	70
Stevanović, Jelena N.	jelena@nanosys.ihtm.bg.ac.rs	55

Stevanović, Magdalena M.		4
Stevanović, Marija	marija.stevanovic@tmf.bg.ac.rs	14
Stevanović, Milena		6
Stojadinović, Stevan		66
Stojanović, Dušica		61
Stojanović, Goran		63
Stojanović, Jovica		75
Stojanović, Srna		66
Stojković Simatović, Ivana		39, 57, 72
Stojkovska, Jasmina		6, 8
Supić, Ivan		72
Szafran, K.	klaudia.wozniak@poczta.umcs.lublin.pl	3
Šavikin, Katarina		16
Šekuljica, Nataša		20
Šćepanović, M.		64
Škorić, Branko		62, 63
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Štrbac, Svetlana		57
Tadić, Nenad B.		24, 32, 55
Tančić, Pavle		60
Terek, Pal		62, 63
Terek, Vladimir	vladimirterek@uns.ac.rs	62, 63
Terpiłowski, Konrad		28, 17
Tomić, Nina	nina.tomic@itn.sanu.ac.rs	4
Tošić, Dragana		9
Tošić, Katarina	tosickatarina32@gmail.com	27
Trajković, Vladimir		2
Tsegelskaya, A. Ya.		76

Uskoković, Petar		61
Uskoković-Marković, Snežana		37
Vasić, Milica M.	mvasic@ffh.bg.ac.rs	52
Vasilić, Rastko		66
Vasiljević, Zorka Ž.		24, 32
Vasiljević-Radović, Dana		55, 71
Veljović, Đorđe		12, 13, 14, 15, 75
Vesely, Jozef		10
Vićentić, Teodora	teodora@nanosys.ihtm.bg.ac.rs	54
Višić, Bojana		68
Vlahović, Filip		26
Vlahović, Jovana	jovana.vlaha@gmail.com	47
Vučković, Kristina		23
Vujančević, Jelena		24, 70
Vujković, Milica		52, 53
Vukmirović, Nenad		50
Vukoičić, Olivera	oliveravukoicic.olja@gmail.com	20
Vukovic, Marina		29
Wiącek, Agnieszka Ewa		3, 5
Woźniak, Klaudia		5
Zemkova, Maria	maria.zemkova@mff.cuni.cz	10
Zheludkevich, Mikhail L.		66
Zhou, Yiqun	YXZ431@miami.edu	41

